Using Computational Fluid-Dynamics (CFD) for the Evaluation of Tomato Puree Pasteurization: Effect of Orientation of Bottle.

A. R. Lespinard[*1,2] and R. H. Mascheroni[1,3]

[1]Centro de Investigación y Desarrollo en Criotecnología de Alimentos, La Plata, Buenos Aires, Argentina
[2]Facultad de Ciencias Agrarias y Forestales, UNLP, La Plata, Buenos Aires, Argentina
[3]Facultad de Ingeniería, UNLP , La Plata, Buenos Aires, Argentina
*Corresponding author: CIDCA - 47 y 116, (B1900AJJ), La Plata, Argentina, alelespinard@yahoo.com.ar

Abstract: Little is known about the temperature and velocity profiles during the thermal processes of liquid foods, which results in over-dimensioned processes to guarantee safety, decreasing the product quality. For this purpose, Computational fluid-dynamics (CFD) offers a powerful tool for numerical predictions of the transient temperature and velocity profiles during natural convection heating of packed liquid foods. The aim of this work was the development of a model that allows to predict the effect of orientation of package on temperature distribution, flow pattern, position of slowest heating zone, processing time and quality changes in tomato puree during pasteurization. It was observed that among the different orientations, the lowest processing time was obtained for the horizontal orientation, while that no difference was found between the process times for the conventional and inverted orientations. Therefore, the lowest loss of quality, quantified by *C-value*, was achieved when the bottle was horizontally positioned.

Keywords: Computational Fluid Dynamics (CFD), Tomato Puree, Pasteurization, Orientation of Bottle

1. Introduction

Pasteurization is one of the oldest known food preservation techniques, based on the partial thermal degradation of microorganisms and denaturation of enzymes, which present potential risk for food spoilage [1]. Industrial processes of pasteurization have to ensure the prolongation of food lifetime, while on the other hand the quality of product should be preserved. The accomplishment of both purposes depends on process conditions which assured the adequate temperature course during process, where consideration of the temperature profile within the product is of great importance [2]. Temperature time history may be derived by using direct measurements or by mathematical modeling [3]. Because of the complex nature of heat transfer in natural convection heating, the determination of the slowest heating zone (SHZ), which is defined as the location in the food receiving minimum heating, is a difficult task [4]. The placement of thermocouples to record the temperature at various positions in a container during heating disturbs the flow patterns. Errors in temperature measurements may occur due to the presence of thermocouple wires, which may restrict the free movement of the liquid [5]. Also, it is difficult to measure the temperature at the SHZ because this is a region, which keeps moving during the heating progress [6]. For this reason, there is a growing interest towards the predictions of temperature distribution during the thermal treatment of liquid foods using CFD modeling.

On the other hand, the characteristics of liquid flow inside the container during heating are a function of its geometry and orientation and even small alterations can result in differences in the process [7]. However, little attention has been devoted on modifications in the orientation of its packaging [8, 9].

Based on the above, the objective of this work was evaluate the effect of orientation of container on temperature distribution, flow pattern, position of SHZ, processing time and quality changes in tomato puree during pasteurization, using CFD.

2. Mathematical Model

2.1. Problem Description

The evaluated problem is the natural convection heating of tomato puree packaged in glass bottle during pasteurization. The models were formed by three parts (glass bottle, liquid food and headspace), which physical properties are described in Table 1.

For liquid food, the properties of a pseudoplastic fluid involving 0.85 % w/w sodium carboxy-methyl cellulose (CMC) solution were used in the simulation model. Steffe *et al*. [10] suggested that this model could be applicable to tomato puree.

Viscosity model:

Food materials are highly non-Newtonian in nature with the flow behavior index typically less than one. The viscosity model selected is given by Christiansen and Craig [11] as:

$$\mu = \mu_0 exp(\frac{nE_0}{RT})\dot{\gamma}^{n-1} \qquad (1)$$

,where the values of constants are given in Table 1. The shear rate ($\dot{\gamma}$) is included in the model despite the usual practice of assuming that shear rate anticipated in the natural convection heating is low (zero shear) and thus the viscosity can be assumed to behave as that of a Newtonian fluid [12] However, when the computed shear rate was lower than 0.01 s^{-1}, the value of μ was calculated using a shear rate of 0.01 s^{-1}.

Table 1: Thermo physical properties used in the simulation model.

Material	Property	Value	Source
CMC (0.85 % w/w)	ρ (kg m^{-3})	950	Varma and Kannan [8]
	C_p (J kg^{-1} K^{-1})	4100	
	k (W m^{-1} K^{-1})	0.7	
	β (K^{-1})	0.0002	
	μ_0 (Pa s^n)	0.002232	
	E_0 (kJ kg mol^{-1})	30.74 10^3	
	n	0.57	
Glass	ρ (kg m^{-3})	2449	Incropera and De Witt [13]
	C_p (J kg^{-1} K^{-1})	750	
	k (W m^{-1} K^{-1})	1.4	
Air	ρ (kg m^{-3})	0.361	Pinho and Cristianini [14]
	C_p (J kg^{-1} K^{-1})	1964.95	
	k (W m^{-1} K^{-1})	0.023	

2.2. Governing Equations

The problem is described by Navier-Stokes Transport Equations. These equations describe mass conservation (continuity law; Equation 2), momentum (Newton's second motion law; Equation 3) and energy (first Thermodynamics law; Equation 4).

Continuity equation:

$$\nabla \cdot \mathbf{v} = 0 \qquad (2)$$

Momentum equation:

$$\rho\left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right] = -\nabla p + \mu\nabla^2\mathbf{v} + F \qquad (3)$$

Energy conservation equation:

$$\rho c_p\left[\frac{\partial T}{\partial t} + (\mathbf{v}\cdot\nabla)T\right] = k\nabla^2 T \qquad (4)$$

Boussinesq approximation is applied for density in the body force (F) as follows:

$$F = -\rho_{ref}\beta(T - T_{ref})g \qquad (5)$$

Initial and boundary conditions:

- Uniform initial temperature (20°C);
- Velocity of the fluid convection currents are null at t=0;
- Velocity of fluid convection currents on the packaging walls are null (no slip condition);
- As boundary condition, packaging heating was considered to be uniform and the medium temperature was boiling water (100°C) with infinite heat transfer coefficient assumption.

2.3. Assumptions used in the numerical simulation

To simplify the problem, the following assumptions were made: (i) Axial symmetry was considered for vertical positions of bottle, which reduces the problem from 3D to 2D; (ii) symmetry in the longitudinal plane was assumed for horizontal orientation, which reduces the domain to only a half of it; (iii) heat generation due to viscous dissipation is negligible, this is due to the use of highly viscous liquid with very low velocities; (iv) Boussinesq approximation is valid; (iv) essential boundary conditions were considered and the effect of surface heat transfer coefficient was neglected; (v) the condition of no-slip on the inner wall of the glass bottle is valid; (vi) the resistance to heat transfer of metallic lids is negligible; (vii) the headspace was considered as a conductive layer of saturated air and (viii) the thermal properties of the glass bottle, air and fluid are constant.

2.4. Mesh details

The boundary layer occurring at the heated walls and its thickness are the most important parameters for the numerical convergence of the solution. Temperature and velocities have their largest variations in this region. To adequately resolve this boundary layer flow i.e. to keep discretization error low, the mesh should be optimized and a large concentration of grid points is needed in this region. If the boundary layer is not resolved adequately, the underlying physics of the flow is lost and the simulation will be erroneous. On the other hand, in the rest of the domain where the variations of temperature and velocity are small, the use of a fine mesh will lead to increases in the computation time without any significant improvement in accuracy. Thus a non-uniform grid system is necessary to resolve properly the physics of the flow. Therefore, unstructured meshes with 5987 and 6361 elements were developed for conventional and inverted vertical positions, respectively. On the other hand, a mesh with 265569 elements was employed to discretize the 3D domain of horizontal position. In all cases, the mesh independence of numerical results was tested successfully.

2.5. Numerical solution

The system of non-linear partial differential equations has been solved by finite element method, using the software Comsol Multiphysics®. For this, a time-dependent solver (BDF) with the direct solver (MUMPS) was employed. The numbers of degrees of freedom in the simulation models were 88882, 96639 and 3947241 for conventional, inverted and horizontal positions, respectively. For a pasteurization process of 7000 s, the simulations take about 3.5, 5 and 516 minutes for conventional, inverted and horizontal positions, respectively. The simulation models were run on an Intel Core i5 PC (Windows 7, 3.2 GHz, 8 GB RAM).

2.6. Determination of the pasteurization times

Pasteurization time was determined on the basis of the SHZ temperature. Then, the time it takes that point to reach an accumulated lethality ($F_{93.3}^{8.3}$) of 5 min was calculated as recommended for those products of high viscosity and acidity such as tomato puree [15]. Accumulated lethalities were calculated in the usual way, by means of Eq. 6, as the integral of the lethal rate L along the processing time.

$$F = \int_0^t L dt = \int_0^t 10^{(T-93.3)/8.3}\, dt \qquad (6)$$

2.7. Determination of quality changes

To evaluate an average deterioration of quality parameters in tomato puree, the average cooking value (C_{ave}) was determined by numerical integration (Eq. 7), using the simulated temperatures for the food domain (Ω) obtained through the simulation model. A reference temperature (T_{ref}) of 100 °C and a thermal resistance factor (z_c) of 33 °C were considered for estimations. The value of z_c was chosen as the average of those values corresponding to the deterioration kinetics of foods quality parameters [16].

$$C_{ave} = \int_0^{t_p} \left(\frac{\int_\Omega 10^{\frac{T(t,\Omega)-T_{ref}}{z_c}} \partial\Omega}{\int_\Omega \partial\Omega} \right) \partial t \qquad (7)$$

3. Results and Discussion

Figures 1a, 1b and 1c shows predicted velocity vectors and temperature profiles for the conventional, inverted and horizontal orientations, respectively, after 75, 570, 1005, 1500, 2010 y 3000 s of process. The lengths of the arrows represent magnitude of the velocities and arrowheads represent the direction. The temperature profiles show that, at the beginning of heating (t=75 s), the heating process is governed by conduction. As heating progresses, the mode of heat transfer changes from conduction to convection. This phenomenon is due that, when the liquid gets in contact with the wall, temperature raises leading to a density decrease. Due to this uneven distribution of density, buoyancy forces are produced and make the liquid move.

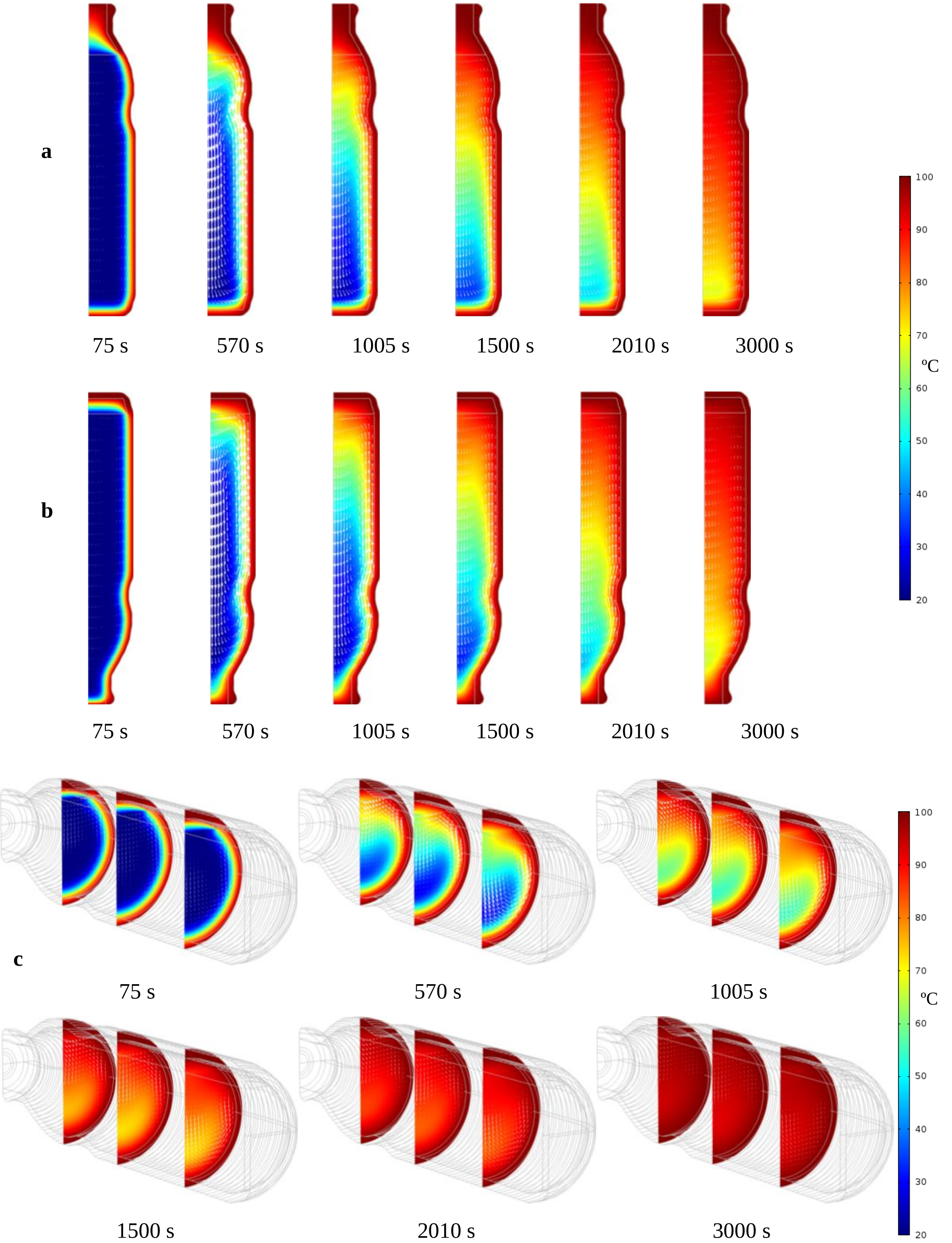

Figure 1. Velocity vectors and temperature profiles for a) conventional b) inverted and c) horizontal orientations, at different times.

The buoyancy force produces an upward flow near the wall. The rising hot liquid is deflected by the lid, and then it travels radially towards the centre of the jar. Thus, a recirculating flow is created. Consequently, the SHZ in the bottle is not a stationary region in the liquid undergoing convection heating. The SHZ moves from the geometric centre to the heel of the bottle and then towards the wall, due to the effect of recirculating flow.

The position of SHZ, at the end of thermal process, was located on the vertical axis of symmetry, at 9 and 17% of the bottle height for conventional and inverted orientation, respectively. These observations are in agreement with those reported by Augusto and Cristianini [18], who reported values from 5 to 20% height for the pasteurization of beer in glass bottle. In the case of horizontal orientation, the position of SHZ is located at 40% of the bottle height and 30% of the bottle diameter.

Figure 2 shows the change in vertical velocities, at mid-height, with time for the three orientations. At the beginning, the magnitude of the velocity vectors increased with time, but as heating progressed the velocity decreased.

This variation of velocity can be explained in terms of the Grashof number (*Gr*) (Eq. 8), which represents the ratio of the buoyancy force to viscous force and its magnitude is indicative of laminar, transition and turbulent flow regimes in natural convection.

$$Gr = \frac{g\beta\Delta T L^3 \rho^2}{\mu^2} \qquad (8)$$

As heating progresses, a more uniform temperature is reached, reducing the buoyancy force in the liquid and leading to a significant reduction of velocity. Temperatures at all points tend to reach the temperature of the heating medium, and consequently the buoyancy forces disappear. *Gr* was estimated considering the height of the bottle, maximum temperature difference and the minimum viscosity in the domain. Thereby, the maximum values of *Gr* obtained were 1651 (t=510 s), 1504 (t=555 s) and 1158 (t=285 s) for conventional, inverted and horizontal positions, respectively. The low *Gr* numbers during the entire thermal treatment validate the laminar flow assumption.

A similar behaviour was evidenced during the evolution of velocities with time for the three orientations, and their magnitudes were found to be in the order of 10^{-4}-10^{-5} ms^{-1}. However, in this Figure, significant differences in the magnitudes of vertical velocities can be observed between vertical and horizontal orientations.

The results indicate that the vertical velocities developed in the horizontal position were lower than those of vertical orientations.

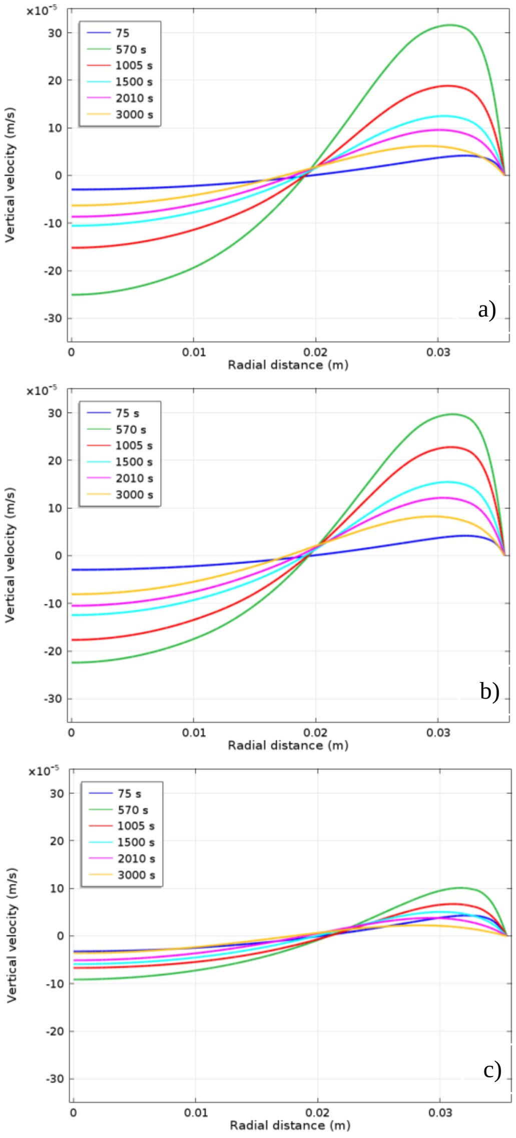

Figure 2. Vertical velocity at mid-height vs. radial position for a) conventional, b) inverted and c) horizontal orientations, at different times.

This is due to that vertical displacement distance of the fluid in the horizontal orientation is lower, since the bottle diameter is smaller than its height.

Figure 2 also shows that the distance between the location of the stagnant region and the wall, named thickness of the ascending liquid, was about 20 mm for all analysed orientations. These values are in agreement with those found by Kumar and Bhattacharya [12] Ghani *et al.* [17], reported values of 15-16 mm and 16-20 mm, respectively, for the same liquid packaged in metal can, though under constant boundary conditions (121 ºC).

The variation of pasteurization time and Cooking value with the orientation are compared in Table 2.

Table 2: Pasteurization times and Cooking values for the different orientations.

Orientation	Pasteurization time (s)	Cooking value (C_{ave}) (min)
Conventional	5625	37.20
Inverted	5625	36.53
Horizontal	2970	19.92

From Table 2, it is evident that the horizontal orientation is found to be most effective among the three orientations considered for pasteurization of tomato puree in glass bottle. The time taken for the SHZ to reach the accumulated lethality ($F_{93.3}^{8.3}$) of 5 min for horizontal orientation was 47% lower than that of the vertical orientations, whereas no difference was found between conventional and inverted vertical orientations.

Consequently, this reduction in processing time obtained by horizontal position, resulted in a decrease quality losses, which were quantified through the average cooking value (C_{ave}).

These results suggest that the horizontal position could be considered as an interesting alternative of processing to conventional vertical position in order to reduce the processing time and improve the quality of tomato puree packaged in bottle.

4. Conclusions

The model developed allowed predict the effect of orientation of package on temperature distribution, flow pattern, position of SHZ, processing time and quality changes in tomato puree during pasteurization. It was observed that among the different orientations, the lowest processing time was obtained for the horizontal orientation, while that no difference was found between the process times for the conventional and inverted orientations. Therefore, the lowest loss of quality, quantified by *C*-value, was achieved when the bottle was horizontally positioned. The results obtained demonstrate the potential of using Computational Fluid-Dynamics (CFD) to evaluate thermal processes of liquids foods, such as tomato puree pasteurization. Moreover, the model developed can also be used to determine which set of operating conditions would enhance the quality and the safety of the final product, thus minimizing expensive and time-consuming pilot test-runs.

5. References

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7. Appendix

Table 3: Nomenclature

C_p	specific heat (J kg^{-1} K^{-1})
CMC	carboxy-methyl cellulose
E_0	activation energy (kJ kg^{-1} mol^{-1})
g	acceleration due to gravity (m s^{-2})
k	thermal conductivity (W m^{-1} K^{-1})
L	lethal rate
n	flow behaviour index
P	pressure (Pa)
R	gas constant (kJ (kg mol)$^{-1}$ K^{-1})
SHZ	slowest heating zone
t	time (s)
T	temperature (ºC or K)
z_c	thermal resistance factor (ºC)
ρ	density (kg m^{-3})
Ω	domain
u	velocity in vertical direction (m s^{-1})
v	velocity in radial direction (m s^{-1})
β	thermal expansion coefficient (K^{-1})
μ	apparent viscosity (Pa s)
μ_0	consistency index (Pa s^n)
$\dot{\gamma}$	shear rate (s^{-1})