Numerical simulation of transient temperature profiles for canned apple puree in semi-rigid aluminum based packaging during pasteurization

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Abstract Pasteurization of canned apple puree was simulated for a 3-D geometry in a semi-rigid aluminum based container which was heated from all sides at 378 K. The computational fluid dynamics code Ansys Fluent 14.0 was used and the governing equations for energy, momentum, and continuity were computed using a finite volume method. The food model was assumed to have temperature-dependent properties. To validate the simulation, the apple puree was pasteurized in a water cascading retort. The effect of the mesh structures was studied for the temperature profiles during thermal processing. The experimental temperature in the slowest heating zone in the container was compared with the temperature predicted by the model and the difference was not significant. The study also investigated the impact of head space (water–vapor) on heat transfer.

Keywords Pasteurization · Apple puree · Slowest heating zone · Ansys Fluent 14 · Mesh structure

Nomenclature

CFD Computational fluid dynamic
 C_p Specific heat (J/kg K)

DSC	Differential scanning calorimeter
F	Thermal death time (min)
H	Height of the can (mm)
k	Thermal conductivity (W/m K)
L	Length of the can (mm)
P	Pressure ($N\ m^{-2}$ or Pa)
R_c	Radius of the container (mm)
R_b	Radius of the spindle (mm)
SHZ	Slowest heating zone
S_M	Source term for momentum
t	Heating time (s)
T	The predicted or measured temperature in the coldest point of the can (K)
T_w	Can wall temperature (K)
T_{ref}	Reference temperature
u, v, w	Velocity components in the x, y, z directions (m/s)
x	Radius at which the shear rate is to be calculated (mm)
z	The temperature required to change thermal death time by a factor of 10
β	Thermal expansion coefficient (K^{-1})
γ	Shear rate (s^{-1})
μ	Apparent viscosity (Pa s)
ρ	Density (kg/m^3)
τ	Shear stress (Pa)
ω	Angular velocity of the spindle (rad/s)

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Introduction

Based on the product processed and the required shelf life, thermal processing could be carried out in two ways. In the first method, heat is applied to a filled sealed container and in the second method, the sterilization of products is carried out outside the final container (Leaper and Richardson

1999). Pasteurization is one of the oldest food preservation techniques, which is based on partial thermal degradation of microorganisms and denaturation of enzymes, which pose a potential risk of food spoilage. Industrial processes of pasteurization have to ensure prolongation of food shelf life while preserving the quality of the product. Accomplishment of both these purposes depends on the process conditions. These conditions can ensure an adequate temperature course during the process, where the temperature profile within the product is of great importance (Plazl et al. 2006).

Heat penetration rate is influenced in canning by container shape, product viscosity, retort temperature, head space of container, and rotation rates (Erdogdu and Tutar 2012). Several studies have been conducted on the mathematical modeling and numerical simulation of can sterilization processes based on different shapes of the container, kinds of foods and effect of rotation speed. Datta and Teixeira (1988) presented transient flow and temperature patterns through numerical simulation of a can uniformly heated on all sides. Zechman and Pflug (1989) investigated the influence of medium properties as well as the size of metal containers on the location of the slowest heating zone (SHZ) of the canned media. Engelman and Sani (1983) reported the results of numerical simulation of pasteurization of beer in glass bottles. Kumar et al. (1990) and Ghani et al. (1999) carried out CFD based transient numerical simulations of the natural convective heating process in the model liquids, carboxy-methyl cellulose and water. Ghani et al. (2002a, b) investigated the effect of rotating a horizontal can at 10 rpm in the thermal sterilization of viscous orange-carrot soup. Garrote et al. (2006) studied the effect of temperature, rotation speed and headspace on heat transfer coefficients of canned green peas during end-over-end sterilization using the response surface method. Boz et al. (2014) investigated the effects of time step size, mesh refinement and choice of numerical solver scheme on temperature and velocity field evolution in a natural-convective heated canned water sample. Geometry modifications are used to increase the rate of heat transfer from the boundary sides to the SHZ (Varma and Kannan 2006). Vatankhah et al. (2016) investigated the effect of geometry simplification of wrinkled wall semi-rigid aluminum containers in heat transfer simulation and the results showed that wrinkled walls do not play an important role in increasing the heat transfer.

Validation is an essential part of the modelling process and the yardstick for success is the level of agreement that can be attained between numerical predictions and experiments (Xia and Sun 2002). In order to generate more reliable CFD data sets for benchmarking simple model approaches, more realistic and accurate

physical properties of the products must be used. In particular, the temperature dependencies of these physical properties (such as thermal expansion and viscosity) need to be quantified more accurately (Chen et al. 2005).

The problem encountered by food processors is to provide adequate heat treatment to ensure that the slowest heating zone within a container receives the critical heat for a specific period of time to inactivate the detrimental effect of microorganisms while maintaining sensory and nutritive properties. The slowest heating zone (SHZ) does not have a fixed location in the enclosure; it changes with time and the geometry of the enclosure (Kannan et al. 2006). Accurate measurement of the temperatures inside the can undergoing thermal treatment is difficult because the probes disturb the temperature–velocity fields. Furthermore, the slowest heating zone is not fixed at one location (Ghani et al. 2002a, b; Kumar et al. 1990). Since the semi-rigid aluminum packaging has recently been introduced to the market, there is limited information about the temperature distribution during the heating process of such containers. Vatankhah et al. (2015) carried out a heat transfer simulation and retort program adjustment for thermal processing of a wheat-based food in semi-rigid aluminum containers. However, no study has addressed heat transfer in thermal pasteurization processes in semi-rigid aluminum containers filled with apple puree. The present study is an attempt to evaluate the thermal process and establish the shape of the SHZ for a fluid food with high viscosity (apple puree) in aluminum-based semi-rigid containers during all pasteurization steps. In addition, the effect of different mesh sizes of semi-rigid aluminum containers on heat transfer and temperature distribution of the food container was investigated and compared to the experimental temperature at the probe position. The thermal death time (F value) was estimated and adjusted to design an optimum production system of apple puree. The effect of head space in the heat transfer mechanism was also studied.

Materials and methods

Experimental procedure

Semi-rigid aluminum-based packaging, Alupak product type B116 made in Switzerland, was used in this study to test the accuracy of the numerical method as explained in the following parts. The can was composed of very thin layers of rotogravure print, stove lacquer white aluminum foil, adhesive (aromatic polyurethane) and polypropylene film with a total thickness of 125 μm and a very low thermal resistance. The length (L) of the can bottom was

71 mm while the length of the can top was 79.4 mm and its height (H) was 24 mm. There was an angle of 95° between the can bottom and side walls. Apple puree (Brix ~ 35), representing the non-Newtonian viscous fluid, was purchased from Aida International Food Industries for experimental measurement of the temperature changes. A needle type-K thermocouple was located in the can ($X = 0$ mm, $Y = 15$ mm, $Z = 12$ mm). The condensing steam was assumed to maintain a constant temperature of 378 K at all boundaries. The can was filled with 100 gr of apple puree (pH = 3.9), providing a headspace of 3 mm and sealed at 553 K by the Alcan machine. The initial product temperature was 297.3 K. Then the experiments were carried out in water cascading Barriquand steriflow (Roanne) retort and the can was put in an upright position. The product was uniformly heated, held, and cooled according to the retort temperature (Fig. 1). The thermocouple was attached to the Ellab data logger CTF9004 with PT100 cables, and the temperature changes were recorded at 60 s intervals. The experiments were performed in Chika International Food Industries, Mobarake industrial zone, Iran.

Mathematical model

Evaluating a mesh independent solution is mostly experience-based, helping to develop an objective and easy to use criterion (Wang and Zhai 2012). The three-dimensional geometry was designed according to the actual container in the design modeler environment. Skin/Loft method was used for generating the volume of the model. The unstructured tetrahedron mesh was generated with a patch independent algorithm since this approach created a more natural shape (Fig. 2).

In the first step, the objective was to see the effect of the mesh structures on the temperature profiles during the thermal processing. The number of the minimum size

Fig. 1 A typical heating, holding and cooling curve of a fluid according to retort temperature

limits of the node and elements are presented in Table 1. Three mesh sizes (0.9, 1 and 2 mm) were examined and the model was respectively divided into 439,743, 326,985, and 41,888 nodes. A grid study was carried out to ensure the solution was independent of the grid size. The root mean square of error (RMSE) presented in Eq. (1) was calculated to compare the simulated and experimented temperatures (at the probe position).

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (T - T_{simulation})^2} \quad (1)$$

In the second step, the objective was to compare the position of SHZ in the model with air headspace and the model with water–vapor headspace. The mesh structure of 2 mm minimum size was used in these simulations and the headspace of 3 mm was once assumed to be filled with air and once with water vapor.

The can outer surface (top, side walls, and bottom) temperatures were assumed to reach the retort temperature. The natural convection heating of the apple puree was simulated for 3000 s. It took 12 time steps to achieve the first 720 s of the heating (come-up time), another 11 time steps for the next 660 s (holding time), and the last 27 time steps to reach the remaining 1620 s of the thermal processing (cooling time). The retort temperature at each minute was applied to the boundary condition of the can (outer surface) in each time step. The solutions were obtained using a variety of time steps and the results depicted the time-step independent of the solutions.

All simulations were performed using a finite volume method (FVM) based on the fluid flow solution. The software used to solve the problem was FLUENT 14.0.0 with 3D, double precision, pressure-based, laminar flow and

Fig. 2 Tetrahedron meshes on 3D model of the Alupak type 116B container

Table 1 Comparison between different meshes

Min size limit (mm)	Number of element	Number of node
0.9	2,558,273	439,743
1	1,891,948	326,985
2	233,318	41,888

natural convection, installed on a P.C. with Intel® Core™ i3-2330 M, CPU @ 2.20 GHz, 4.00 GB RAM with a 2009 Microsoft Corporation Windows 7 Home Premium, 64-bit Operating System (Service Pack 1). The computer processing time spent was about 10 h for simulating the heat transfer in the different meshes. A preset convergence limit of 1×10^{-5} was used for the continuity and momentum equations and 1×10^{-8} for the energy equation. Unsteady-state laminar flow and time steps of 60 s were envisaged during the heating and cooling cycle. The semi-implicit method for pressure-linked equations consistent (SIMPLEC) was used for the pressure velocity coupling scheme. This method leads to a smoother convergence for the pressure equation. The pressure interpolation was performed using the standard method. In spatial discretization, Green-gauss node based was used for gradients. Second order upwind method was employed for the momentum and energy interpolation. The number of iterations in this study was 100 to achieve more convergence. The under-relaxation factors were adjusted to smaller than 1 to get a good convergence of the numerical solution.

Governing equations and boundary conditions

The simulations were performed by CFD analysis, using the Ansys Workbench 14.0 program (Ansys Inc., USA) to simultaneously solve the Navier–Stokes and energy equations. The partial differential equations governing the natural convection motion of the fluid in the 3D can include continuity, energy conservation and momentum equations in x, y and z coordinates as shown below. These equations can be found in details in Versteeg and Malalasekera (2007).

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0 \quad (2)$$

Energy conservation:

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} = \frac{k}{\rho C_p} \left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right] \quad (3)$$

Momentum equation components in three dimensions (x, y and z): x, y and z components of momentum equation:

$$\rho \frac{Du}{Dt} = \frac{\partial(-p + \tau_{xx})}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + S_{Mx} \quad (4)$$

$$\rho \frac{Dv}{Dt} = \frac{\partial(-p + \tau_{yy})}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{zy}}{\partial z} + S_{My} \quad (5)$$

$$\rho \frac{Dw}{Dt} = \frac{\partial(-p + \tau_{zz})}{\partial z} + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + S_{Mz} \quad (6)$$

The CFD model described above was performed with the following initial and boundary conditions, assuming that the can was filled up to the top with 3 mm head space. The boundary conditions used include $T = T_w$, $v = 0$, $u = 0$, and $w = 0$. The initial product temperature was supposed to be $T = 297.3$ K. To simplify the problem, the following assumptions were made (Ghani et al. 2001):

1. Heat generation arising from viscous dissipation is negligible; this is due to the use of a highly viscous liquid with very low velocities.
2. The assumption of no-slip condition at the inside wall of the can is valid.
3. The thermal boundary conditions are applied to the food liquid boundaries rather than the outer boundaries of the package. This is true since the can is composed of a very thin layer with a total thickness of less than 0.1 mm and has a very low thermal resistance. However, the rise in the retort temperature is measured and used in the simulation in present study.
4. As the condensing steam commonly used in the thermal processing has a high thermal heat transfer coefficient; the side walls, the bottom and the top surfaces are supposed to have a constant temperature during the heating time.

Thermal and physical properties

Viscosity, density, specific heat and thermal conductivity values of the apple puree were necessary for the solution of the equations. The shear rate would be small due to the extremely high viscosity of the food used in this simulation, which has been verified by viscosity measurement at different shear rates. Hence, viscosity can be assumed independent of shear rate and the fluid behaves as a Newtonian fluid.

The viscosity of the product was measured as a function of the temperature from 313 to 353 K using a Brookfield viscometer (DV III ULTRA) with spindle number 64 (Ahmed and Ramaswamy 2006). The shear Rate was determined to be 0.4291 s^{-1} using Eq. (7) (Ghani et al. 1999).

$$\gamma = \frac{2\omega R_c^2 R_b^2}{x^2(R_c^2 - R_b^2)} \quad (7)$$

Table 2 Properties of the experimental food system

System properties	Equations as function of temperature	R ² (correlation coefficient)
Viscosity (μ)	$\mu = 0.1183T^2 - 22.885T + 1271.7$	0.9
Specific heat (Cp)	$Cp = 8.0363T + 3276.1$	0.99
Thermal conductivity (k)	$k = 0.0093T + 0.5249$	0.99
Density (ρ)	$\rho = -0.3769T + 1153$	0.98
Coefficient of volume expansion (β)	$\rho = \rho_{ref}[1 - \beta(T - T_{ref})]$	

The specific heat and thermal conductivity were estimated by the mass fraction of their constituents (water, protein, fat, ash and carbohydrate) (Sahin and Sumnu 2006). The density was measured by a pycnometer at seven temperature steps. The thermal properties of this food system are presented in Table 2. The thermal expansion coefficient was calculated as $2.82 \times 10^{-4} \text{ K}^{-1}$ based on the equation in Table 2 (Bejan 1993).

Steffe and Ford (1985) suggested that a fluid involving 0.85 % w/w sodium carboxy-methyl cellulose (CMC) solution in water is applicable to tomato puree, carrot puree, green bean puree, applesauce, apricot and banana purees, which are regularly canned and preserved by heating. For validation, this experimental system was characterized for apple puree, which illustrated a good agreement with the aforementioned studies.

The experimental results for the viscosity, specific heat and thermal conductivity expressed above were applied with the piecewise-linear method in the material part of the software.

Calculation of the F value and model validation

The thermal death time “F” is the time required to cause a stated reduction in the population of microorganisms or spores (Sun 2012). Calculation of F values requires knowledge of time–temperature recordings at the slowest heating point in the can. This value is commonly obtained using a thermocouple connected to a recording potentiometer (Robertson and Miller 2007). The pasteurization effect value was extracted from Eq. (8), where T_{ref} and z for *Bacillus polymyxa* are 100 and 8.8 K respectively, and T is the retort temperature (Larousse and Brown 1997).

$$F = \int_0^t 10^{(T-T_{ref})/z} dt \quad (8)$$

Statistical analysis and software

Ansys Workbench 14 software was used to construct the geometry and grid and CFD software package (Fluent 14) was used to carry out the computations. Studentized t test

was used to compare the predicted and experimented data ($p < 0.01$).

Results and discussion

This study was an attempt to investigate natural convection heating of a can filled with apple puree at horizontal position and heated by condensing steam at 378 K from all sides in a 3D geometry. The evolution of the temperature profile with the heating time for all the three grids are shown in Fig. 3. The RMSE values for 439,743, 326,985 and 41,888 nodes (0.9, 1, and 2 mm according to the interval mesh size, accordingly) were respectively 1.25, 1.211 and 1.203 until the end of the holding time (1380 s). This small error indicates the validity of the simulation results. The predicted temperature did not change by increasing the number of the nodes. The temperature difference of the three meshes was not significant as the studentized t test indicated ($p < 0.01$). Computational time is one essential factor to determine usefulness of a CFD solution for possible design and optimization studies. Using finer meshes dramatically increases computational costs (Boz et al. 2014). To reduce the computations volume and save computer energy and time, the mesh with 41,888 nodes (having the least RMSE) was used for further simulation. The location of the coldest point of SHZ was

Fig. 3 Experimental temperature at the probe position and theoretical predicted temperature in the can for different meshes at $t = 23$ min

Table 3 Comparison of SHZ position in Cartesian system in two meshes

Time (s)	Fine mesh (1 mm) (X, Y, Z)	Coarse mesh (2 mm) (X, Y, Z)
720	(−0.43, −0.43, 11.89)	(−0.95, −0.95, 11.65)
1440	(−0.43, −0.43, 11.89)	(−0.95, −0.95, 11.65)
1680	(−2.99, −2.99, 11.89)	(−2.85, −2.85, 11.65)

Fig. 4 Experimental measurements at the sensor position and theoretical prediction of temperature in the can ($X = 0$ mm, $Y = 15$ mm, $Z = 12$ mm)

presented in the Cartesian system in Table 3 for the two meshes.

The models were validated by comparing the predicted average temperature values at the probe position (point P) in the modeled container ($X = 0$ mm, $Y = 15$ mm and $Z = 12$ mm) and the experimented temperatures during the process time. Studentized t test was used to compare the predicted and experimented data. The results showed a high similarity between the predicted and experimented values at point P ($p < 0.01$). Obviously, both predicted models (air headspace and water–vapor headspace) were in good agreement with the experimented models (Fig. 4).

The results of the simulation illustrated in Fig. 5 show the shape of SHZ for the plane of $X = 0$ from the can bottom for the different heating and cooling periods during the pasteurization.

In the present study the variation of the geometric center temperature with time was compared to the probe point. Ghani et al. (2002a, b) reported that the location of SHZ for a can filled with carrot-orange soup lying horizontally covers the whole cross-sectional area of the can at the early stages of heating while it migrates towards the bottom of the can and as the secondary flow at the bottom of the can pushes the SHZ closer to the center of the can. The SHZ developed into an ellipse shape after a short period of heating (Ghani et al. 2002a, b). Vatankhah et al. (2015) indicated that SHZ for semi-rigid containers containing

Haleem was located at the geometric center of the container. *Haleem* is a common food used as a breakfast dish, baby food, and a special dish during Ramadan and Muharram, the holy Islamic months, cooked in a wide geographical zone from Iran to Bangladesh (Sajjad 2011). The shape of SHZ was similar for the two predicted models in this study. As shown in Fig. 5, the SHZ shape varies with time and becomes very small at 1380 s (the end of the holding stage of the pasteurization) and settles around the center of the puree mass. At the end of the holding stage of the process ($t = 1380$ s), the maximum velocity was 4.73×10^{-6} m/s and the location of SHZ remained fixed near the center of the puree mass.

Earlier analyses conducted on sterilization of foods such as canned tuna, thick syrups, purees, and concentrates were assumed to be through conduction heat transfer only (Kannan et al. 2006; Kumar et al. 1990). The results obtained by both convective and conductive modes of heat transfer are compared with the fictitious base of heat transfer by mere conduction in order to evaluate the importance of the convective in pasteurization of a highly viscous substance like the one used in this study. The model food can be assumed to be heated by conduction as the SHZ position was at the geometric center of the container (Kannan et al. 2006).

If the container is supposed to be completely filled with apple puree (a model without headspace), SHZ will occupy a larger volume at $t = 120$ s than the model with headspace (Fig. 6). In the rest of the processing time, the headspace did not influence the position and shape of SHZ because of the high heat transfer coefficient of the water vapor in the headspace.

The coldest point (at the end of the heating period) in the model without headspace was selected to be studied for pasteurization efficiency ($X = -0.95$, $Y = -0.95$ and $Z = 11.65$) (Fig. 7). The pasteurization effect value during the heating process is presented in Fig. 8, indicating 7.96 min as the total F_0 . The F_0 was compared to tomato paste with $F_0 = 5$ min (Westport 1968). The time–temperature was adjusted to reach a lower F_0 value by using Simpson’s rule for numerical approximation of the integration (Holdsworth and Simpson 2008; Alonso et al. 2013). The results showed that the product would reach a logical sterility of about $F_0 = 4.96$ min, by a 3 min reduction in the heating period.

Fig. 5 The temperature contours of plane $X = 0$ mm, a_1 and a_2 at $t = 720$ s (end of come-up time), b_1 and b_2 at $t = 1380$ s (end of holding time), c_1 and c_2 at $t = 3000$ s (end of cooling time), *left* and *right* figures are air headspace and water-vapor headspace respectively

Fig. 6 The temperature contours of plane $X = 0$ mm at $t = 120$ s **a** without headspace, **b** water-vapor headspace

Fig. 7 The coldest point in model without headspace ($X = -0.95$, $Y = -0.95$, $Z = 11.65$ mm) at the end of holding time ($t = 1380$ s)

Fig. 8 Pasteurization effect value in the coldest point of model without headspace

Conclusion

A mathematical model was developed and experimentally validated to study the temperature distribution and pasteurization efficiency of an aluminum-based semi-rigid container containing apple puree. Additional different meshes illustrated no significant effect on the temperature distribution. The measured temperatures at the central point in the can were compared with those predicted by the models and found to be in good agreement with each other. The CFD-based model showed that the position of SHZ was located in the geometric center of the puree mass. The results of the simulation showed that the headspace has a significant effect on shape and location of SHZ in early stages of heating. In order to improve the nutritional value of the product, the time–temperature profile was adjusted to achieve the desired pasteurization.

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Compliance with ethical standards

Conflict of interest There is no conflict of interest.

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