Iranian Food Science and Technology Research Journal
Vol. 14, No.6, Feb. Mrch. 2019, p. 113-125

نشریه پژوهشهای علوم و صنایع غذایی ایران
جلد 14، شماره 6، بهمن - اسفند 1397، ص. 113-125

Numerical Calculation F-value and Lethality of Non-Newtonian Food Fluid during Sterilization based on Can Geometry

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Received: 2018.01.26
Accepted: 2018.08.13

Abstract:

Amount of heat transfer temperature was stimulated in the slowest heating zone of 3.5% starch dispersion during canning sterilization with 10% headspace. The computational fluid dynamics software COMSOL 4.1 was used and governing equations for energy, momentum, and continuity were computed using a finite volume method. The effect of container geometry (cylinders with 6*10cm and 10*6cm dimensions, and cones with 10 cm height and 5 cm radius on 0 and 180° position) on heat penetration parameter (j) and microbial lethality (L) in slowest heating point were investigated. The temperature of the slowest heating zone was monitored by a thermocouple and then compared with the predicted temperature by software. It was determined that cone-shaped container had the fastest heat transfer during sterilization. Also, container geometry has a significant effect on slowest heating zone shape, position, final temperature, j, L, and F-value.

Keywords: Microbial lethality, Numerical calculation, Sterilization, Container geometry, Heat penetration parameter

Introduction

Canning is one of the economical sterilization methods for food preservation (Karaduman, Uyar *et al.* 2012). In canning industries, in order to prevent the overcooking and preserving the quality of the product, the estimation of good sterilization method is necessary (Karaduman, Uyar *et al.* 2012). The industrial sterilization process is based on a temperature-time profile which ensures the product shelf life and quality by deactivating the special microorganism or enzyme and reducing the loss of nutritional factors in the product. Heating rate and heat transfer mechanism in canned foods (conduction and convection) depends on several factors like difference between retort and product temperature, the ratio of surface to volume, product viscosity (Tattiyakul, Rao *et al.* 2002) package shape, and rotation rates. Several studies have numerically investigated the factors affecting on slowest heating zone (SHZ) shape, position and temperature profile during sterilization of canned foods. Datta and Teixeira (1988) numerically predicted the velocity and temperature of canned water in static retort and suggested that cold area is donate-like and is near one-tenth length from the bottom (Datta and Teixeira 1988). Kumar *et al.* (1990) also used finite element method to simulate non-Newtonian food heating in vertical metal cans which were heated from the top at 121˚C (KUMAR, Bhattacharya *et al.* 1990). They realized that in natural convection, the cold area is near the bottom of the can. Wiese and Wiese (1992) used different numerical methods for determining the break point (WIESE and WIESE 1992). Ghani *et al.* (1999) numerically simulated the natural convection of canned water and CMC with PHOENICS and predicted the fluid flow and internal temperature of these model fluids. They found cold area moves to the bottom during the heating process and its size and shape is different in water and CMC (Ghani, Farid *et al.* 1999). Ghani *et al.* (2002) also studied the sterilization of canned orange soup. They found the temperature of cold area reaches a maximum temperature of 107˚C and SHZ moves to the bottom due to natural convection and stay in 20-25% (Ghani, Farid *et al.* 2002). Farid and Ghani (2004) used a

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DOI: 10.22067/ifstrj.v0i0.71219

new computational technique to estimate the sterilization time of canned foods. In order to predict the temperature profile of the cold area and natural convection in the can, they used computational fluid dynamics with PHOENIX. They suggested that due to little vertical dimension the effect of natural convection in a horizontal can is lower than vertical can (Farid and Ghani 2004). Dimou and Yanniotis (2011) predicted temperature and velocity profile of 7.6*10.9 cm cans containing 4% brine and 0, 1, 8 and 19 asparaguses. They found the cold area is near the %13.5 from the bottom and is not dependent on asparagus numbers (Dimou and Yanniotis 2011). Dimou *et al.* (2011) studied the effect of process variables on temperature profile, flow patterns, and location of the cold area in static cans with computational fluid dynamics. They used asparagus, olive in %4 brine, and peach in %20 sucrose in 76*109 mm cans and have found the flow and temperature are affected by shape, type and arrangement of particles inside the can, and properties of the filling fluid (Dimou and Yanniotis 2011). Srghini and Erdogdu (2016) investigated the effect of rotation rate (end-over-end) and viscosity (water and 1.5% CMC) on heat transfer characteristics of a canned food with headspace (Sarghini and Erdogdu 2016).

The mechanism of unsteady convection is very complex and a valid modeling is essential to determine heat process requirements to predict temperature during heating. In order to make more realistic data from CFD modeling, more accurate conditions are required. The shape, situation, and temperature of SHZ is strongly depended on package geometry, heating time, and product viscosity (Abdul Ghani and Farid 2006, Kannan and Sandaka 2008, Kumar, Wee *et al*. 2012). Since most of the food fluids are non-Newtonian and they have a complex behavior during heating, different studies were done to simulate heating rate in such model liquids such starch dispersions. During the heating, process starch makes a viscose paste (Lagarrigue and Alvarez 2001) that the heat transfer mechanism changes from convection to conduction. This phenomenon leads to a slope change in time-temperature curve at a determined time known as a breakpoint (X_{bh}) (Yang and Rao 1998) (Fig. 1). Due to break in the heating curve, these fluids are known as broken heating fluids. There is limited information about the effect of container geometry on heat penetration parameters of SHZ in starch distribution. However, no study has addressed the numerical calculation of heat penetration parameters and microbial lethality during starch sterilization in its real canning state with headspace. The present study is an attempt to evaluate different container geometry on heat penetration parameters and microbial lethality of starch dispersion SHZ during static sterilization.

Materials and methods

Experimental Procedure

Starch dispersion (3.5% w/w) was filled in two cylinders (6*10 cm and 10*6 cm) and one cone (10 cm height and 5 cm radios) with equal volumes. In real canning procedure there is a headspace above the product and according to Ranjbar *et al.* (2016) the SHZ is near the air-product interface, the T- type thermocouple was placed in 2 cm below the air-product interface (Ranjbar, Ziaiifar *et al.* 2015, Ranjbar, Aman Mohammad *et al.* 2016). All measurements were performed in triplicates. The 8-port data logger (Pico-TC08, England) and related software (PicoLog) were used to record the temperature data with 10s intervals. The steam was assumed to maintain a constant temperature of 394.14 K at all boundaries. The initial temperature of starch dispersion was 323.14 K.

Governing Equations

Since starch dispersion is a breaking heating fluid, the equations (1-6) were used to represent the apparent viscosity of 3.5% starch dispersion as a function of temperature (Yang and Rao 1998):

Viscosity increase section in 78-89.5˚C:

$$\eta \times \left(\frac{\omega}{\omega_r}\right) = 7.4 \times 10^{-6.0} \left(\frac{T}{100-T}\right)^{6.208} \quad (1)$$

The end of viscosity increase (pick

viscosity) and the beginning of viscosity reducing in 89.5-92.5˚C (2):

Reducing viscosity in 92.5-121˚C (3):

Since ω and η^* are dynamic shear data, in order to relating them to static shear data ($\dot{\gamma}$ and η_a), modified Cox-Mers rule is used (4) (Barnes, Hutton *et al.* 1989, Yang and Rao 1998).

C and α shift factor at 25˚C are equal to 2.07 and 1.01, respectively. Thus we have Eq. (5): η^* (T) is as Eq. (6):

T is temperature (°C) and if $T\text{-}x \geq 0$ then $H(T-x)=1$ and if $T\text{-}x \leq 0$, then $H(T-x)=0$

$$\eta * \left(\frac{\omega}{\omega_r}\right) = -69122.86 + 2244.36T - 24.28T^2 + 0.088T^3 \tag{2}$$

$$\eta * \left(\frac{\omega}{\omega_r}\right) = 4.11 + exp\left[23298.3\frac{1}{T} - \frac{1}{366.1}\right] \tag{3}$$

$$\eta * (\omega) = C\left[\eta_a(\dot{\gamma})\right]^{\alpha} \tag{4}$$

$$\eta_a = \left[\frac{1}{2.07}\eta * (T)\left(\frac{\dot{\gamma}_r}{\gamma}\right)\right]^{\frac{1}{1.01}} \tag{5}$$

$$\begin{aligned}\eta * (T) = {} & \left(7.4 \times 10^{6.3}\left(\frac{T}{100-T}\right)^{6.203}\right) \times [H(T-50) - H(T-89.5)] \\ & + (-69122.86 + 2244.36T - 24.28T^2 + 0.088T^3) \times [(H(T-89.5) - H(T-95)] \\ & + \left(4.11 + exp\left[23298.3\frac{1}{T} - \frac{1}{366.1}\right]\right) \times [(H(T-95) - H(T-121)]\end{aligned} \tag{6}$$

Other physical and thermal characteristics of 3.5% starch dispersion is shown in table 1:

Table 1- Starch dispersion heat characteristics (Yang and Rao 1998)

Quantity	Parameter	Equation	Unit
Density	rho	1000*(1-0.00053*(T-IT))	[kg/m^3]
Conduction transfer coefficient	k	0.66	[W/(m*K)]
Special heat coefficient	Cp	4180	[J/(kg*K)]
Convection transfer coefficient	h	Nu_starch*k_starch/(h)	

Numerical simulation was includes pairing two physical phenomena: heat transfer and fluid flow. Since the system was cylindrical and cone shaped cans containing food with natural convection, non-isothermal laminar flow equations were used. For each problem, one 3-D geometry was defined and meshing was done according table 2.

Table2- Different cans meshes for cone 0°, cone 180°, cylinder1, and cylinder2 geometries

Can Characteristics	Number of element	Maximum element size
Cone 0 °	61,549	0.0335
Cone 180 °	61,549	0.0335
Cylinder1 (6*10cm)	54,680	0.039
Cylinder2 (10*6cm)	107,356	0.0201

A BDF[1] method for time stepping and Backward Euler to time discretization were used. The system used to run the test and solve the equation was IntelVR CoreTM i5CPU M 460 @ 1.70 GHz and 6GB RAM.

The governing equations for non-isothermal laminar flow for domains were defined. The equations of continuity (7), energy (8), and momentum (9) are as below:

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla . (\rho u) = 0 \qquad (7)$$

Energy equation:

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p u \cdot \nabla T = \nabla \cdot (k \nabla T) + Q + Q_{vh} + W_p \qquad (8)$$

Momentum equation (9).

$$\rho \frac{\partial u}{\partial t} + \rho (u \cdot \nabla) u = \nabla \cdot \left[-pI + \mu (\nabla u + (\nabla u)^T) - \frac{2}{3} \mu (\nabla \cdot u) I \right] + +F \qquad (9)$$

Where *P* is the static pressure, *U* is velocity field, *T* is Temperature, *μ* is viscosity, *ρ* is density and *F* is the external body force including gravitational effects. To simplify the problem, following assumptions was used (Farid and Abdul Ghani 2004, Abdul Ghani and Farid 2006, Erdoğdu 2008, Kannan and Sandaka 2008, Dimou, Stoforos *et al.* 2011, Dimou and Yanniotis 2011, Erdogdu and Tutar 2012, Kumar, Wee *et al.* 2012):

Data related to cooling phase were ignored.

Effect of gravity (9.8 m/s) was expressed as a body force.

The estimation of food density as a function of temperature for Bostwick calculation for starch was used.

Fluid was considered homogeneous.

Heat Penetration and Lethality Analysis

Since in thermal diffusion analysis, the formula methods are correct than empirical methods (Yang and Rao 1998), formula methods were used in this study for calculating *j* parameter. The smallest *j* indicates there is less time required to reaching the uniform heating. The accuracy of these calculations was evaluated using CFD (Wang and Sun 2003). The parameter of J_h index, as a dimensionless correction factor, is calculated by the Eq. (10):

$$j_h = \frac{T_\infty - T_m}{T_\infty - T_i} \qquad (10)$$

Where T_∞ is steam temperature (121°C), T_m is temperature at time=t (s), and T_i is initial temperature of product. Since pH of starch dispersion is 6, the goal of sterilization is based on reduction or deactivation of *C. Botulinum* spores. Lethality (L) in coldest point was according to Eq. (11):

$$L = 10^{(T-121.1)/10} \qquad (11)$$

Where, 121.1°C is the reference temperature and T is the predicted or measured temperature in the coldest point of the can and z is the temperature required to change thermal death time by a factor of 10 that is 10 °C.

The F value for a process is the number of minutes required to kill a known population of microorganisms in a given food under specified conditions. This F value is usually set at 12 D values to give a theoretical 12 log cycle reduction of the most heat-resistant species of mesophilic spores in a can of food. For example, if there were 10,000 spores of a species of spore in a can of food and a 12 D process was given, the initial 10,000 spores (10^4 spores) would be reduced to a theoretical 10^{-8} living spores per can, or again, in theory, one living spore per 10^8 cans of product (one spore per one hundred million cans). F-value is calculated according to Eq. (12):

$$F = \Delta t \times \sum L \qquad (12)$$

Where t is time (s). All these parameters were calculated for two different holding time at 121.1°C at 15 min (900s) and 20 min (1200s) after heating by 121.1°C assumed vapor (tables 3 and 4, respectively).

Results and Discussion

Model validation

The predicted and experimental temperature of SHZ was shown in Fig. 2. Differences was not significant using T student test ($P<0.05$).

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[1] Backward Differentiation Formula

The (r) of experimental and simulated data was 0.9484 and the root mean square of errors (RMSE) was 0.124°C. It shows the good accuracy between experimental and model temperature data during CFD modeling.

Heat transfer analysis

Calculation of heat penetration parameters and microbial efficiency is critical to study the uniformity of heat transferring in canning industry (Smout, Ávila *et al.* 2000, Smout, Loey *et al.* 2000). But these calculations are a little complex in non-Newtonian fluids. Starch dispersion is a non-Newtonian solution that has a viscosity dependent on the temperature. By increasing the time and temperature of the heating process, the starch granules start to swelling and then gelatinization (Lagarrigue and Alvarez 2001). Before gelatinization, the heat transfers convectively and after gelatinization, due to conductive heating, the rate of heat transferring and temperature profile is change (Fig. 1).

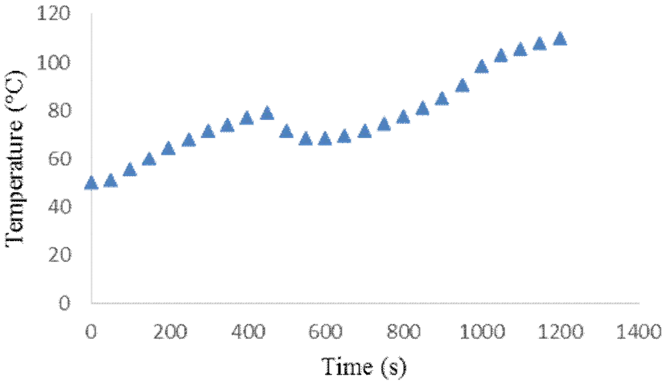


Fig. 1. Temperature-time profile of 3.5% starch dispersion during sterilization (the situation of X_{bh} is determined as 450s or 7.5 min)

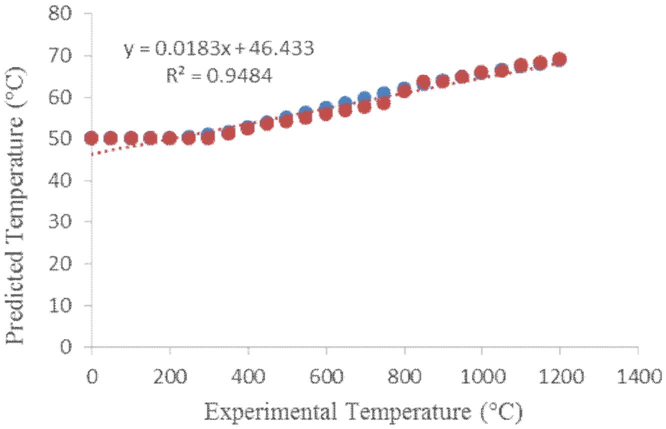


Fig. 2. Comparison of experimental and predicted temperature of starch dispersion SHZ

As can be seen in Fig, 1, the conduction heating leads to a delay in temperature increase. These changes in viscosity significantly affect the heat transfer mechanism. In order to simulation, the temperature profile of such fluids, the simulation of the effect of viscosity on SHZ position, shape, and temperature is necessary (Sarghini and Erdogdu 2016). Calculation of heat transfer parameters in combination with viscosity changes and container geometry is a complex phenomenon (Varma and Kannan 2005, Buckow, Baumann et al. 2011). Fig. 3 shows the significant effect of geometry on the slowest heating point of different studied geometry.

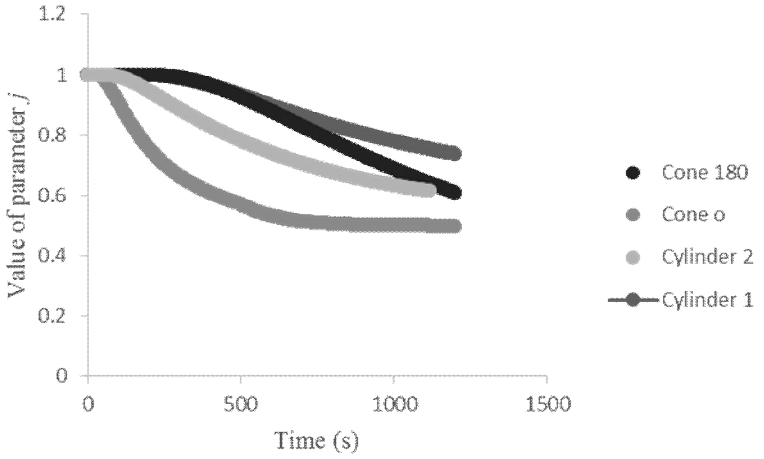


Fig. 3. Values of parameter *j* for different container geometries

The cone 0° shows a good reduction in j by heating time. It indicates the time required for uniform heating in cold point is low in cone 0° (Tutar and Erdogdu 2012). But the cylinder 1 has a relatively higher j parameter than other. It may be due to the higher height of container that fluid should rise doing convection heat transferring. It is however because of the low velocity of starch dispersion during heating (about 0- 65×10^{-8} (m/s)) that increase the time of starch movement before its gelatinization begins to start (Yang and Rao 1998, Lagarrigue and Alvarez 2001). It also has an effect on L and F. As can be seen from tables 3 and 4, the L, F, and temperature of SHZ (0, 0, 7,5) of cone 0° is higher than other geometries; both at the end of 15 min or 20 min holding time.

Table 3- The heat penetration parameter *j* and Lethality factor at 15 min (900s) after reaching the container wall to 121.°C for different container geometry filled with IT=50°C of starch dispersions

Can Characteristics	j_h	Temperature of SHZ (°C)	L	F (min)
Cone 0°	0.4999	85.5	0.0195	0.293
Cone 180°	0.731	69.07	0.00017	0.0025
Cylinder1 (6*10cm)	0.803	63.9	0.00008	0.001
Cylinder2 (10*6cm)	0.652	74.7	0.00096	0.014

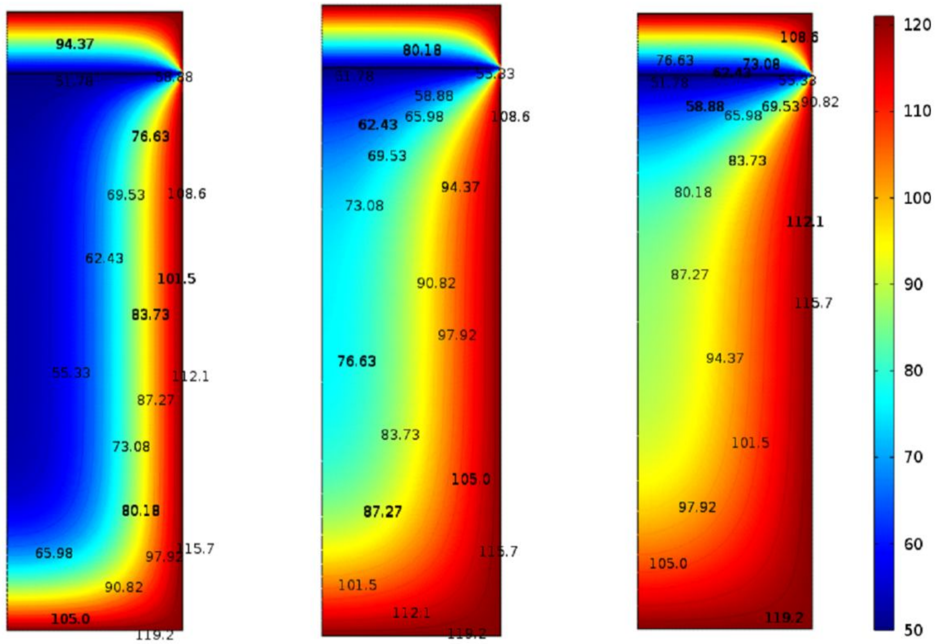
Table 4- The heat penetration parameter *j* and Lethality factor at 20 min (1200s) after reaching the container wall to 121.°C for different container geometry filled with IT=50°C of starch dispersions

Can Characteristics	j_h	Temperature of SHZ (°C)	L	F (min)
Cone 0°	0.496	85.72	0.0323	0.646
Cone 180°	0.608	77.78	0.00086	0.0172
Cylinder1 (6*10cm)	0.735	68.8	0.0003	0.006
Cylinder2 (10*6cm)	0.613	77.45	0.0024	0.048

When the starch temperature is 75°C (viscosity increasing section is at 78-89.5°C (gelatinization phase) (Yang and Rao 1998)), its viscosity increase with temperature increasing. The layers near the wall are slowly gelatinized and heat transfers gently from gelatinized layers to other (Yang and Rao 1998).

Figures 4-7 shows the temperature- time profiles of 4 studied geometries at 15 and 20 min holding times. It is interesting that the shape and situation of SHZ are absolutely different in each geometry. The shape of SHZ in cone 0° at time=360s is like an Erlenmeyer flask and with increasing the heating time, two different SHZ with shapes and different temperatures appeared. But finally the SHZ near the air-fluid interface remains and one near the bottom disappears rapidly. This is due to a short height near the cone wall that starch dispersion should rise during convection heating (Ranjbar, Ziaiifar *et al.* 2015, Ranjbar, Aman Mohammad *et al.* 2016).

The holding time during sterilization is critical to destruction the goal microorganism or enzyme and retaining the nutritional materials in foods. At the end of two selected holding time (15 and 20 min), the position of the slowest heating point was determined. The cold point position for cone 0°, cone 180°, cylinder1, and cylinder2 at the end of 900s (15 min) was respectively (0, 0, 8.5 and 0, 0, 1.4), (0, 0, 7), (0, 0, 7.2), and (0, 0, 1.5). And after 1200s (20 min) holding time, was at (0, 0, 8), (0, 0, 8), (0, 0, 8), and (0, 0, 1.8). In cone 0° after 900s, the bottom part of SHZ disappeared and the part near the air-product interface remains. Varma and Kannan (2006) studied the effect of geometry and position of metal container on SHZ. They assumed fulfilled containers. In their study because of the connection of upper wall with the product, the SHZ in cone 180° is at the bottom of the container (Varma and Kannan 2006). But when the air phase is used in a container, the effect of air as a preventing area for direct heat transferring from the wall to the product should be considered.



(a) (b) (c)

Fig. 4. Temperature counters of cylinder 1 at (a) t=360s, (b) t= 900s, and (c) t=1200s

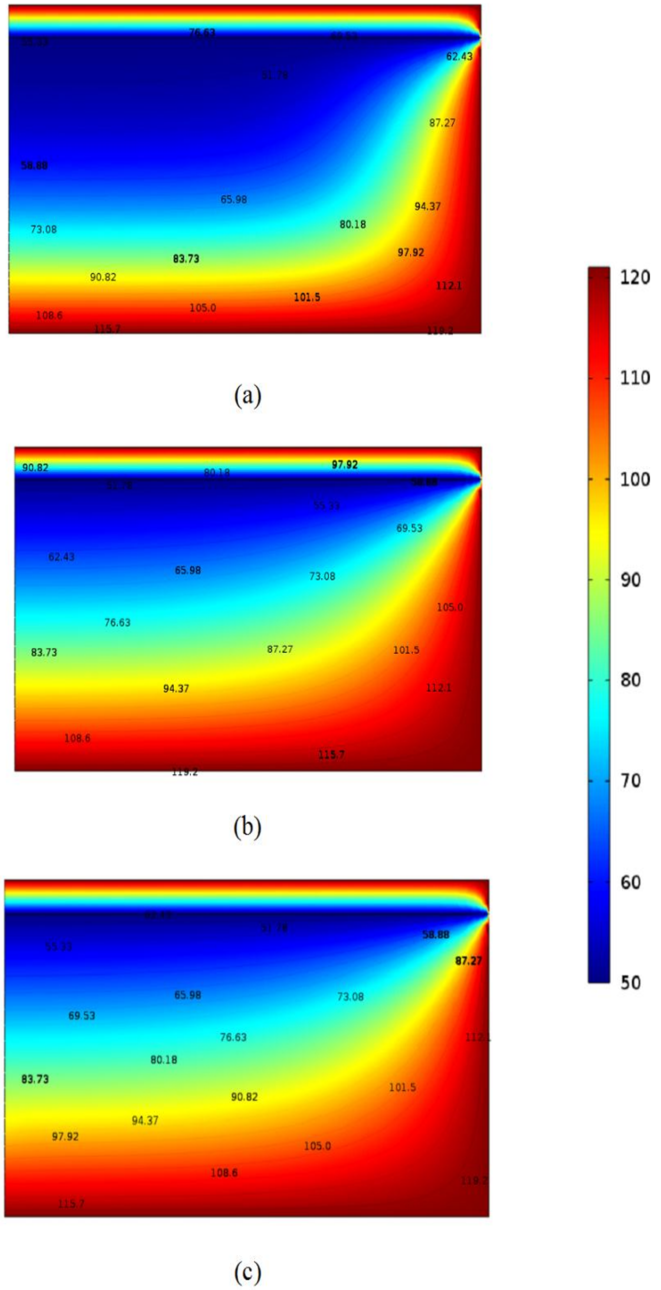


Fig. 5. Temperature counters of cylinder 2 at (a) t=360s, (b) t= 900s, and (c) t=1200s

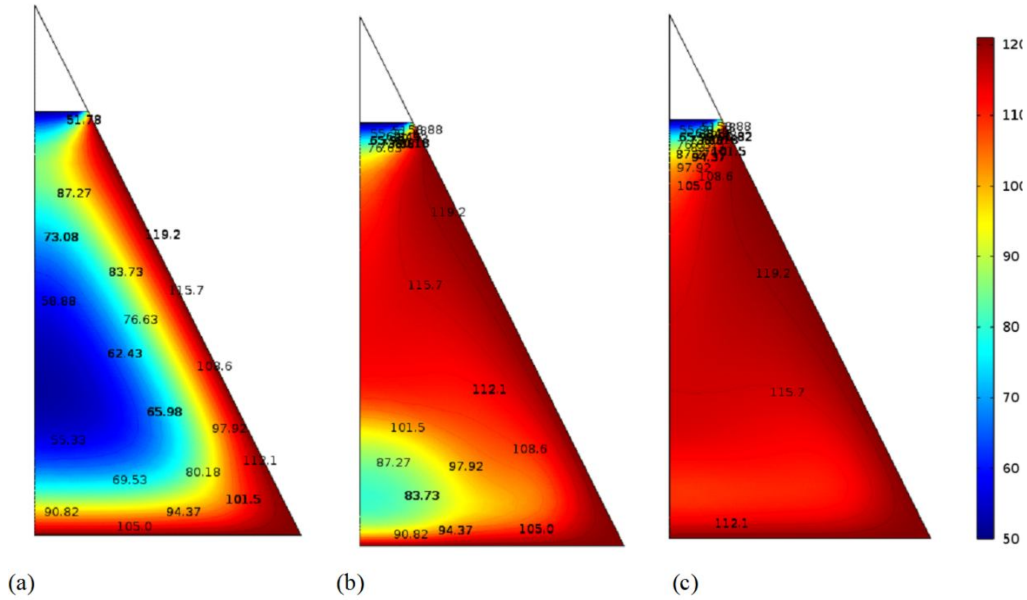


Figure 6- Temperature counters of cone 0° at (a) t=360s, (b) t= 900s, and (c) t=1200s

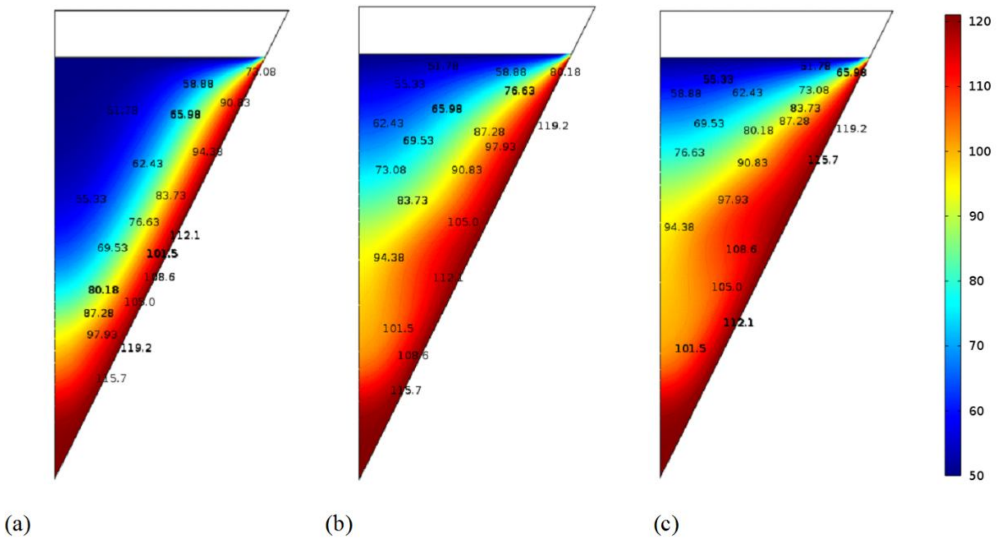


Fig. 7. Temperature counters of cone 180° at (a) t=360s, (b) t= 900s, and (c) t=1200s

In this study, it was demonstrated that at 121.1°C, the 20 min holding time is critical to reaching a good L and F value (tables 3 and 4). The 5 min additional holding time leads to about 1.6, 5, 3.75, and 2 fold on Lethality effect of temperature in cone 0°, cone 180°, cylinder1, and cylinder2, respectively. Also, F-value arises 2.2, 6.8, 6, and 4 fold, respectively. It shows the importance of the selection of a good temperature-time profile during sterilization. But before all, the data showed that the selection of an accurate cold area in heat transfer monitoring is a key step in food sterilization. Because of microbiological and technical considerations, there is a headspace on top of the food product that in stationary sterilizations (such fluids as starch dispersions that high shear rate breaks their structure (Lagarrigue and Alvarez 2001)), has a great effect on place and shape of SHZ and should be considered in heat transfer studies (Varma and Kannan 2005). Ranjbar et al. (2015) studied the role of the headspace on the processing time of 3.5% starch dispersion. They found heating rate was higher in the samples which were fulfilled while when the headspace is used in a container, a larger volume of headspace leads to a faster healing process. The cold area in 100% fill samples is near the 10% length from the bottom of the can. SHZ in samples with 80 and 90% fill levels, is near the air-product interface. In static sterilization of the food metal containers, heat transfer rate in 100% filled cans are more and if there is headspace in the can, the heating rate decrease with decreasing the air volume but the final temperature is higher (Ranjbar, Ziaiifar *et al.* 2015).

Conclusion

A CFD model was developed to study the time-temperature distribution of a 3.5% starch dispersion in different can shapes. The experimental and predicted temperature at SHZ was in a good agreement. CFD modeling showed the container geometry has a significant effect on SHZ shape, position, final temperature, j, L, and F-value. Also holding time at 121.1°C for 20 min leads to a significant decrease in j and increase in F compared with holding time of 15 min. Also numerically demonstrated that in a static metal container which contain fluids with natural convection behavior during the heating process, the SHZ is close to the interface of air-product.

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Iranian Food Science and Technology Research Journal
Vol. 14, No.6, Feb. Mrch. 2019, p. 113-125

نشریه پژوهشهای علوم و صنایع غذایی ایران
جلد 14، شماره 6، بهمن - اسفند 1397، ص. 125-113

محاسبه عددی اندیس F و L سیال خوراکی غیرنیوتنی طی استرلیزاسیون بر حسب هندسه قوطی

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تاریخ دریافت: 1396/12/06
تاریخ پذیرش: 1397/05/22

چکیده

مقدار درجه انتقال حرارت در ناحیه سرد دیسپرسیون نشاسته 3/5 % طی استرلیزاسیون در قوطی دارای 10% سرفضا شبیه سازی شد. از نرم‌افزار محاسبات عددی COMSOL ورژن 4/1 استفاده شد و معادلات مربوط به انرژی، جابه‌جایی، و پایستگی با استفاده از روش حجم محدود حل شدند. اثر هندسه قوطی (استوانه با ابعاد 10× 6/6 × 10 سانتی‌متر و مخروط با ارتفاع 10 سانتی‌متر و قطر 5 سانتی‌متر به شکل عمودی رو به بالا و رو به پایین) بر پارامتر نفوذ حرارتی (*j*) و کشندگی میکروبی (L) در ناحیه سرد بررسی شد. درجه حرارت ناحیه سرد توسط یک ترموکوپل پایش و با نتایج پیش‌بینی شده نرم‌افزار مقایسه شد. مشخص شد که قوطی مخروطی شکل سریعترین انتقال حرارت طی استرلیزاسیون را داراست. همچنین هندسه قوطی اثر معنی‌داری بر شکل، موقعیت، دمای نهایی، پارامتر j، L و F ناحیه سرد دارد.

واژه‌های کلیدی: کشندگی میکروبی، محاسبه عددی، استریلیزاسیون، هندسه قوطی، پارامتر نفوذ حرارتی

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