

Determination of Cold Spot Location for Conduction-Heated Canned Foods Using an Inverse Approach

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Abstract: Cold spot location is a focal point in thermal process lethality calculations for conduction heated canned foods. An inverse heat conduction problem (IHCP) approach was used to model heat transfer for canned food with headspace using a one dimensional heat conduction model. Sequential function specification algorithm was used to solve for heat fluxes history at the can headspace side using known internal transient temperature measurements. The estimated heat fluxes were then used to solve the direct heat conduction problem for the temperature profiles in the axial direction including at the sensor position. Deviations between estimated temperatures and measured temperatures at the sensor position were calculated using root mean square error. From all the treatments used, a maximum error of 0.29 °C was obtained for the whole measurement period of the treatment which is well within thermocouple measurement error. The excellent agreement between the measured and calculated temperatures at the sensor position is an indication of an accurate estimation of heat fluxes and subsequent location of the cold spot. The results revealed that the cold spot is located at about 59 % of the model food height from the bottom of the can for the three levels of headspace investigated (10%, 14% and 20%). The result of this research provides a useful guide for accurate location of cold spot when collecting heat penetration data for conduction heated foods with headspace predominantly occupied by water vapor. This will aid in assuring the safety of canned foods based on accurate calculation of thermal process lethality.

Keywords: Headspace, Lethality, Cold spot, IHCP, Thermal sterilization.

INTRODUCTION

The classical method of evaluating the lethal effect of thermal sterilization process is based on the heat penetration parameters (f_h , f_c , j_h , j_c) proposed by Ball [1]. The heat penetration parameters are often determined from time-temperature measurements at the geometric center of a can which is often assumed to be the slowest heating point (cold spot). The time-temperature at the cold spot can also be determined from numerical solutions of the governing heat conduction equation in cylindrical or other geometries subjected to prescribed boundary conditions. The accuracy of the prediction of the time-temperature history at the cold spot depends on how accurate the prescribed boundary conditions describe the actual thermal process conditions. Different boundary conditions were used by various researchers to solve the heat conduction equation in different geometries for temperatures at any position and time. The boundary conditions of the first type are frequently used for simulating the thermal sterilization process [2-7]. The boundary conditions of the third type are also used in simulating thermal sterilization [8-10]. However, the boundary conditions used by these researchers did not take into consideration the insulating effect of headspace due to lack of information on heat transfer coefficients at the headspace side of a can. However, the data provided by Mohamed [11] for heat transfer coefficients for can

headspace could be useful in describing realistic boundary condition. Other reported studies related to headspace focused on experimental investigation of the effect of headspace on heat penetration parameters and cold spot location for cans [12-14], or for flexible packages and semi rigid containers [15-17]. The cold spot location was reported to shift upward from the geometric center towards the top surface of the food for flexible packages with entrapped air [15, 16] and for semi rigid container [17]. Varga, Oliveira [18] used mathematical modeling to investigate the effect of four processing factors including headspace volume variability on thermal process lethality (F-value). They found that variability of 2.5 % in headspace did not produce any significant effect on the F-value. Recently, Khakbaz Heshmati *et al.* [19] carried out research work to investigate the effect of headspace on cold spot location using numerical solution with convective heat transfer coefficient at the headspace side. They found that cold spot is shifted from the center to the top of the jar for the two level of headspace investigated namely 6% and 10%.

The aims of this research are to present a systematic approach for modeling heat transfer for can with headspace comprise predominantly of water vapor and to determine the location of the cold spot for different headspace sizes.

INVERSE HEAT CONDUCTION ALGORITHM

Estimation of temperature at any position and time from a governing heat conduction differential equation

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and prescribed boundary and initial conditions are known as the direct method. While determination of the boundary conditions, initial condition or thermal properties from transient temperature measurements is known as an inverse heat conduction problem (IHCP). There are several pioneer algorithms proposed for the solution of the IHCP including, the exact matching algorithm [20] the function specification algorithm [21-23] and the regularization algorithm [24]. In the present study the function specification algorithm will be used to solve for the unknown surface heat flux at the headspace side of a can and then the direct problem will be solved for temperature as function of time along the axial direction to locate the cold spot. Since cold spot for cylindrical can is located along the central axis due to symmetry in the radial direction, it is sufficient to consider one-dimensional problem with temperature variation in the axial direction to locate cold spot as the radial direction has no influence on the location of the cold spot. To accomplish the requirement of a unidirectional heat conduction in the axial direction for cylindrical can geometry, the boundary surface normal to the radial direction should be well insulated, this will help in eliminating the term that contain temperature gradient in the radial direction in the Fourier's heat conduction equation. Once the term that contains temperature variation in the radial direction is excluded, the problem will become similar to unidirectional heat transfer in slab geometry. For a can with no headspace, the boundary condition at the top and at the bottom of the can may be identical leading to cold spot at the geometric center of the can. When headspace is present, the boundary condition at the top and the bottom of the can will be different leading to shift in cold spot location from the geometric center along the central axis. The magnitude of the shift depends on the size of the headspace and the composition of gases and water vapor in the headspace. The heat transfer model to conduction canned food with headspace and negligible temperature variation in the radial direction can be expressed as:

$$\rho c \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial z^2} \quad (1)$$

With initial and boundary conditions:

$$\text{at } t = 0 \quad T(0, z) = T_o$$

$$\text{at } z = 0 \quad T(t, 0) = T_h \text{ (bottom of the can)}$$

$$\text{at } z = L \quad -k \frac{\partial T}{\partial z} = q(t)$$

Estimation of the surface heat flux q_m can be obtained from minimization of the following sum of squares function:

$$S_m = \sum_{i=1}^r (Y_{m+i-1} - T_{m+i-1})^2 \quad (2)$$

Where, m is index for discrete time and r number of future time intervals for which heat flux is assumed to have certain functional form. Minimization of the above sum of squares function can be easily performed using different functional form assumption for heat flux for time t_m to t_{m+r-1} such as constant, linear, cubic, parabolic or other form. Using the assumption of constant heat flux Beck, Blackwell [25] developed the following function specification algorithm for calculating heat flux:

$$\hat{q}_m = \hat{q}_{m-1} + \frac{\sum_{i=1}^r (Y_{m+i-1} - T_{m+i-1}) X_{m+i-1, m}}{\sum_{i=1}^r X_{m+i-1, m}^2} \quad (3)$$

Where $X_{m+i-1, m}$ is the sensitivity coefficient defined by

$$X_{m+i-1, m} = \frac{\partial T_{m+i-1, m}}{\partial q_m} \quad (4)$$

From the governing heat conduction equation and the prescribed boundary conditions the following are the equations for the sensitivity coefficients.

$$\rho c \frac{\partial X}{\partial t} = k \frac{\partial^2 X}{\partial z^2} \quad (5)$$

With initial and boundary conditions:

$$\text{at } t = 0 \quad X(0, z) = 0$$

$$\text{at } z = 0 \quad X(t, 0) = 0$$

$$\text{at } z = L \quad -k \frac{\partial X}{\partial z} = 1$$

COMPUTER PROGRAM

A FORTRAN computer program was written to solve numerically equations (1) and (5) based on Crank-Nicolson implicit finite difference discretization.

Equation (3) is also incorporated into the program for calculating the heat flux at each time step. Once the heat flux is known, the problem becomes a direct problem and the program then solves the direct problem for the temperature distribution in the axial direction. The numbers of nodes used were 100 and the time increments were one second. The program can handle different values for the number of future time steps (r).

MATERIAL AND METHOD

Material

Bentonite suspension was used extensively as a model food due to its stability and possibility of preparation of suspensions with different thermo-physical properties. In this research 8% (w/w) bentonite suspension was prepared according to the procedure proposed by Josef *et al* (1996). The thermal conductivity of the suspension was determined using the KD2 thermal conductivity probe ((Labcell Ltd., UK) using three replicates is 0.61 ± 0.01 W/(m- °C). The thermal diffusivity was calculated using the equation proposed by Martens [26]

$$\alpha = [0.057363W + 0.000288(T + 273)] \times 10^{-6} \quad (6)$$

Equation (6) was developed based on more than 200 experimental data and was reported to be more accurate compared to Riedel [27] correlation (Dinçer [28]). The volumetric heat capacity (ρc) was calculated from the thermal conductivity and thermal diffusivity.

Experimental Setup

Can with an effective diameter of 74 mm and height 50 mm was used in this study. The can inner side wall was coated with a thick layer of Silicon gel to retard heat transfer from the radial direction. Three levels of headspace were used mainly, 5 mm (10%), 7 mm (14%) and 10 mm (20%), the percentage refer to the volume of the headspace relative to the volume of the can. These levels of headspace cover the range of 9% to 16.4% reported in previous published work [14, 18, 29]. Once the headspace is known the height of the model food is also known then the cans were punctured and special receptacle was fitted to allow insertion of a hypodermic needle thermocouple type-J at a position of 10 mm below the surface of the model food for all the headspace levels used. Following the preparation of the cans, the prepared bentonite suspension was heated in a kettle using boiling water

bath until the temperature of the bentonite about 80 °C, then poured into the prepared cans, and filled to the desired marked level and carefully vacuum sealed to eliminate all gases using a vacuum seaming machine. Further insulation to the outside of the cans was done by placing the prepared can inside a hollow Styrofoam cylinder with special cut for the receptacle that holds the thermocouple, then all the interfaces between the can and the Styrofoam at the edges were sealed carefully with a silicone gel to prevent water entry to the side of the can. Furthermore, the outer side of the Styrofoam cylinder was wrapped with a shrink polymeric film. The prepared cans were then attached to two Aluminum blocks coated with silicon gel. The purpose of the Aluminum blocks is to provide support for the cans to be in the upright position during immersion in a boiling water bath and to allow the bottom of the can to be exposed to the boiling water. The coating is to minimize the drop in the boiling water upon immersion, details of the experimental setup is shown in Figure 1. The experiments were carried out in duplicate for each headspace with separate run for each headspace size. The short can with small height/diameter ratio was selected for this study because such can will be most sensitive to error in axial position of thermocouple compared to cans with large height/diameter ratio.

Data Collection

For data collection, a hypodermic thermocouple was first attached to a data logger OPTO22 (Solution Engineering SdnBhd, Kuala Lumpur, Malaysia). The data logger was then connected to a computer equipped with a LABTECH version 12.1 software which manages and controls the data collection process. The thermocouple was calibrated using glass thermometer and ice-water mixture. The calibration was verified using boiling water yielding temperature reading of 100 ± 0.1 °C. The thermocouple was then inserted carefully into the can at the set position.

A stainless steel cylindrical container was used to heat about six liters of water using a gas stove. When the water reached agitated boiling stage the prepared can was submerged into the water bath and the data logger was activated to start collecting time-temperature data. The collection of the data was set at 30 second intervals for a period of 15 minutes. The data was stored in the hard disc of the computer for further processing.

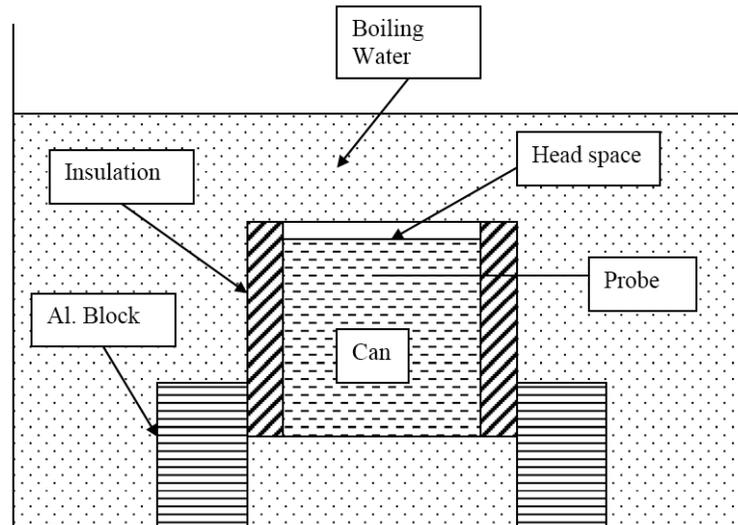


Figure 1: Schematic showing the can experimental setup.

RESULTS AND DISCUSSION

Surface Heat Flux Estimation

The input data to the developed computer program are temperature history data, the position of the sensor, the height of the sample, the thermophysical properties of the food material, time and space step sizes, the known boundary conditions, the temperature measurement intervals and the number of future time intervals (r). Based on this information, the program calculates the heat flux in sequential manner at each time (m). Once the heat flux at the headspace side is known the problem becomes a direct problem. The same computer program then calculates the temperature profile in the axial direction using a subroutine for the solution of the direct heat conduction problem. The accuracy of the calculated heat flux was checked by comparing the calculated temperature at the sensor position with the measured value using the root mean squares error (RMSE) given as:

$$RMSE = \left[\frac{1}{N} \sum_{i=1}^N (Y_i - \hat{T}_i)^2 \right]^{1/2} \quad (7)$$

Restivo and Sousa [30] indicated that by using a root sum square method all the components are combined for producing the combined uncertainty. The value of the number of future time measurements found to yield minimum RMSE value based on preliminary investigation was found to be $r = 4$ for all the treatments. Table 1 shows the RMSE for the different cans used in this study. A maximum value of 0.29°C which is within the allowable error encountered

during temperature measurements by thermocouples was obtained. This represents the combined errors from temperature measurements and numerical computation over the whole measurement time domain indicating the accuracy of the calculated heat flux and the subsequent solution of the direct problem for the temperature distribution in the axial direction. Figure 2 shows comparison between the calculated temperature from the estimated heat flux and the measured temperature at the sensor position for the 14% headspace. It is evident that there is an excellent agreement between these two temperature histories indicating the reliability of the algorithm and the accuracy of the calculated heat flux. Beck, Blackwell [25] investigated different types of function forms for heat flux including cubic, parabolic, linear and constant for the function specification method the authors found that the constant heat flux form resulted in excellent and efficient estimation of the heat flux compared to the experimental heat flux data and the other functional forms.

Table 1: Root Mean Square errors for Different Experimental Run

Run	Headspace (mm)	RMSE ($^\circ\text{C}$)
1	5	0.11
2	5	0.23
3	7	0.21
4	7	0.29
5	10	0.10
6	10	0.16

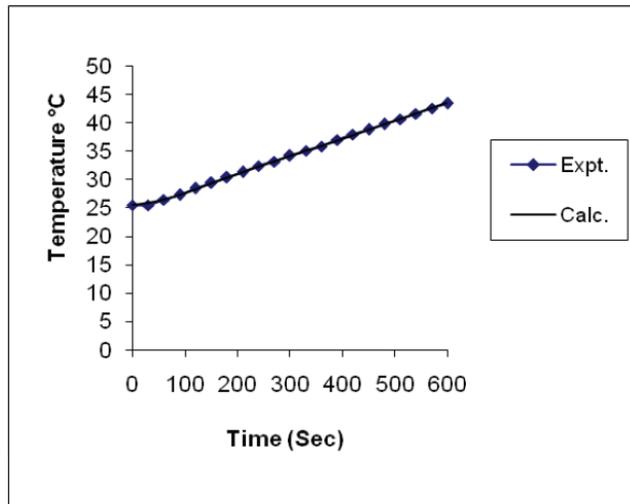


Figure 2: Experimental and calculated temperature profiles at the sensor position for 14% headspace.

Cold Spot Location

Figure 3 to 5 show the temperature profile in the dimensionless axial direction relative to the height of the model food (L). It is clear that the temperature profile is not symmetric for all the three levels (10%, 14% and 20%) of headspace resulting in cold spot at position 59%, 58% and 59% of the model food height, respectively. The unsymmetrical temperature profile is due to the difference in thermal resistance at the bottom and the top of the can. It is important to emphasize that the position of the cold spot for the cans replicates at each headspace levels are identical with slight difference in magnitudes of the temperatures due to the differences in the initial temperature for the different replicates. The reason for the cold spot position being at about a constant value of 59% relative to the model food height irrespective of the size of the headspace indicates that the heat transfer coefficients at the headspace side are close for the three levels. Mohamed [11] found that the effective heat coefficients for headspace of 10%, 14% and 20% consist mainly of water vapor and were 54.2, 53.2 and 50.8 $W/(m^2 \cdot ^\circ C)$, respectively with an average value of 52.73 and standard deviation of ± 1.75 . This indicates that the effective heat transfer coefficients for can headspace comprised mainly of water vapor were not significantly different. The author attributed that to water vapor equilibrium considerations that may result into the same water density and hence same convective effects in the headspace. However, presence of gases and water vapor mixture may produce different results as phase equilibrium in the headspace will depend on pressure, temperature and composition resulting in different thermo-physical property and hence different

convective effect in the headspace. Due to the fact that the effective heat transfer coefficients were similar for the levels investigated here, the shape of the temperature profiles in the axial direction for the three levels of headspaces were not significantly different. Therefore, the cold spot will be at position of 0.59L from the bottom of the can and the magnitude of L depends on the size of the headspace. Figure 6 shows the cold spot position relative to the can height (H). It is obvious that for 10% headspace the cold spot is above the geometric center. As the headspace increased to 14% the cold spot is slightly above the geometric center. For the 20% headspace, the cold spot moved below the geometric center. The trend shown in the figure clearly demonstrated that headspace size influence the position of the cold spot and it could be either below or above the geometric center. However, the results of Figure 6 also showed that cold spot will be at the geometric center for headspace in the range 14 – 20 %. For short cans such as the one used in this study, the height of the food (L) that results in cold spot at the geometric center can be easily calculated from the result of this study using the formula [$L = H/(1.18)$] this correspond to headspace of 15.25% for the can size used in this study. Josef *et al.* [14] carried out heat penetration tests at different axial positions for bentonite dispersion (5g/L) packed in 307 x 409 with different headspace levels. They found that for a headspace of 19 mm which correspond to 16.4 % the cold spot is at the geometric center which is close to the value of 15.25% obtained in this study using a relatively shorter can. Varga, Oliveira [18] showed that for headspace of 10% with variability of 2.5% the effect on process lethality is more relevant for short can (211 x 109 and 307 x 113) compared to tall can (211 x 304 and 307 x 512). Although they indicated that the variability range in headspace investigated did not have very important effects on process lethality compared to the other variables investigated, they acknowledge that headspace might change the exact location of the least lethality point inside the package. Robertson and Miller [13] and Joseph *et al.* [14] found that process lethality at the geometric center of canned bentonite increases significantly with increases of headspace, this suggests that the heat transfer coefficient at the can headspace is not a limiting factor in heat transfer for the range of headspaces investigated which is in agreement with the results of Mohamed [11] which revealed that, the heat transfer coefficients for headspace of 10%, 14% and 20% were not significantly different ($P < 0.01$). This means, that thermal resistance at the can headspace did not increase with increase of the headspace size at least for the range investigated. If heat transfer

coefficient at the headspace decreases with increase of headspace the thermal process lethality at the geometric center would be expected to decrease with increase of headspace due to increase of thermal resistance at the headspace side. Therefore due to the fact that thermal process lethality increases with increase of headspace, one would expect cold spot to migrate along the central axes depending on the size of the headspace. Exact location of the cold spot is very important in optimizing thermal process schedule. Uno and Hayakawa [31] investigated the effect of errors in thermocouple positioning when collecting transient temperature measurements for determination of thermal diffusivity in cylindrical can. They found that a one mm deviation in locations, where the temperatures were monitored, as well as similar deviations in the height and radius of a cylinder resulted in significant variations in the thermophysical property values this will subsequently affect the time-temperature distribution. It is also shown by the previous authors that these variations may be significantly reduced if one uses a cylinder for which height and radius are 100 mm or greater. This clearly indicates that temperatures distribution will be influenced by errors in position as small as 1 mm especially for short cans; therefore it is very important to place the thermocouple exactly at the cold spot when carrying out a heat penetration test to minimize the error in thermal process lethality calculation. Exact positioning of the temperature measuring thermocouples can be achieved using sensors with very small tip with probe attached to a fitting holder affixed to the can wall, many design of such sensor systems are currently available from different manufacturers. However, use of computerized mathematical models will provide accurate prediction of time-temperature at the cold spot if a reliable heat transfer coefficient at the can headspace is provided.

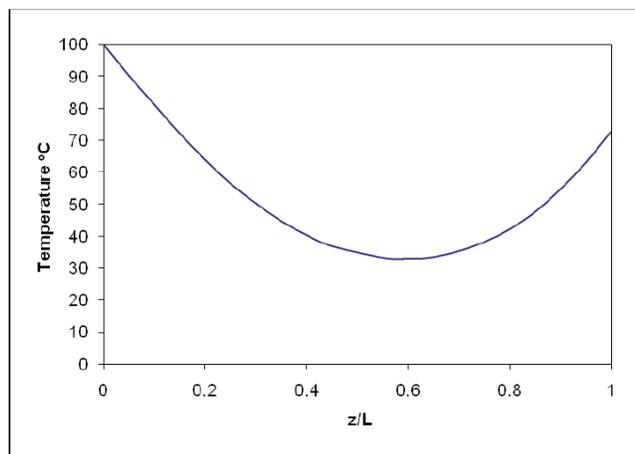


Figure 3: Temperature profile in the axial direction at time 10.5 minutes for 10% headspace.

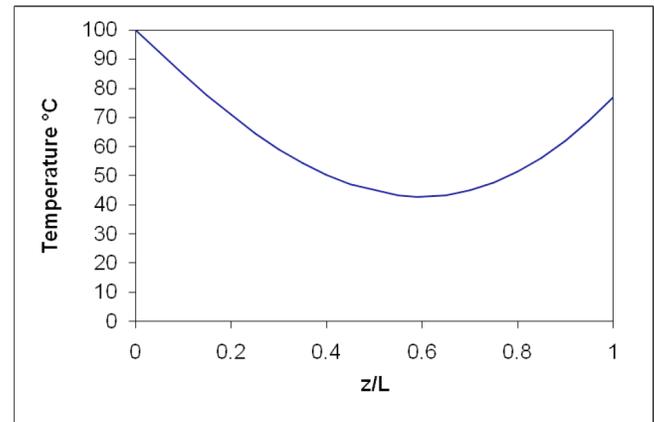


Figure 4: Temperature profile in the axial direction at time 10.5 minutes for 14% headspace.

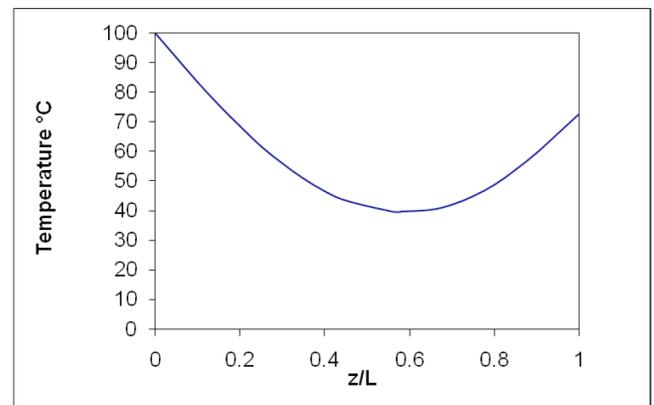


Figure 5: Temperature profile in the axial direction at time 10.5 minutes for 20% headspace.

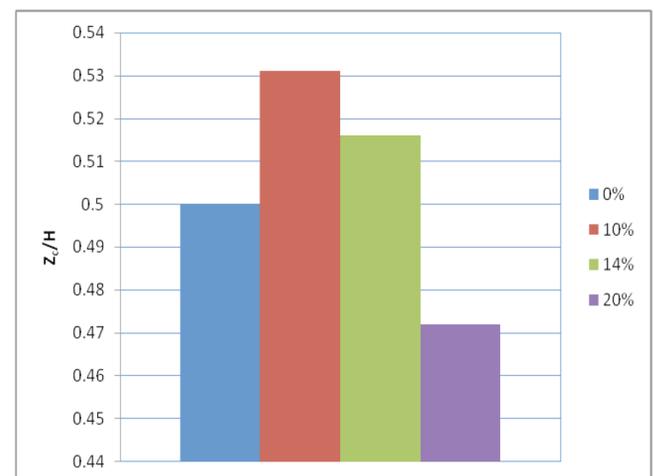


Figure 6: cold spot locations relative to the can height for different percent headspace level.

The results of this research clearly indicates that it is very important to precisely determine the location of the cold spot for can with headspace, as the time temperature data collected at the geometric center may provide less accurate information regarding process

lethality in the presence of headspace. This may have a serious consequences regarding product safety or quality as the geometric center may not be the cold spot at some levels of headspace and that may result in either under processing or over processing depending on the level of the headspace which may have serious effect on consumer health or product quality.

CONCLUSIONS

Heat transfer through can headspace was investigated using an inverse heat conduction approach. The method is based on estimating the boundary heat flux at the headspace side using internal transient temperature measurements. 8 % bentonite suspension packed in cylindrical can with diameter 74 mm and height 50 mm with three levels of headspace 10%, 14% and 20% were used in this study. The accuracy of the calculated heat flux at the can headspace side was confirmed by comparing calculated and measured temperature at the sensor position. Furthermore, the results reveals that the cold spot was located at about 59% of the model food height from the bottom of the can for the three levels of headspace investigated. These results provide guideline for determining cold spot location when collecting heat penetration data to be used for lethality calculation for thermal sterilization process for cans with comparable heights. However, the presence of significant amount of gases in the headspace may yield different results regarding cold spot location.

NOMENCLATURE

c	=	specific heat, J/(kg-K)
H	=	height of the can, mm
k	=	thermal conductivity, W/(m-°C)
L	=	height of the model food, mm
N	=	number of measurements
t	=	time, s
r	=	number of future time steps for function specification
S_m	=	sum of squares function for function specification method
T	=	temperature, °C

T_o = Initial temperature, °C

\hat{T} = estimated temperature, °C

T_h = heating medium temperature (100 °C)

W = fractional moisture content (wet basis)

Y = measured temperature, °C

q = heat flux at the headspace boundary, (W/ m²)

\hat{q} = estimated heat flux at the boundary, (W/ m²)

z = space in the axial position, mm

z_c = cold spot position, mm

Greek

ρ = density, kg/m³

α = thermal diffusivity m²/s

Subscript

i = time index

m = time index

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