Modeling and Simulation of Thermal Sterilization of Conduction Heat Canned Foods Using Heat Transfer Coefficients Boundary Conditions

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Abstract: A generalized computer simulation model for thermal sterilization of conduction-heated canned food was developed. The model is based on expressing the boundary conditions in term of heat transfer coefficients to allow for handling all possible types of boundary conditions in addition of updating the boundary conditions during thermal processing. The developed computer program was based on an alternating direction implicit (ADI) finite difference method using Crank-Nicolson scheme of discretization. The computer simulation model was validated using published experimental time-temperature data collected at the geometric center for 5 % (w/w) canned bentonite in cylindrical can with 9 % headspace. An excellent prediction for the can center temperature during both heating and cooling cycle compared to experimental data was obtained. The program was used successfully in tracing the location of the cold spot by examining the solution of the temperature profiles along the central axial direction at a given time confirming that cold spot for the can size and headspace level used is at the geometric center. The developed computer program will be a valuable tool in thermal process design, scheduling and optimization because it is based on realistic thermal processing conditions that take into consideration actual thermal resistance at the can boundary surfaces and at the headspace side.

Keywords: Thermal sterilization, Modeling and simulation, ADI, Heat transfer coefficients, Can headspace.

INTRODUCTION

Modeling and simulation of food processing unit operations received greater attentions in recent years because it allow optimization related to heat transfer in terms of energy efficiency, equipment design, product safety and quality retention, reduce production cost and improve the product quality and safety [1]. In addition, computer simulation models are very powerful in thermal process design, optimization and online control of process deviations [2-9]. Knowledge of time-temperature data at the cold spot for canned foods is a key requirement in thermal process calculations. In addition, knowledge of cold spot location is important information needed to properly calculate the lethality of a thermal process to ensure can food safety. However, the majority of the published research works for conduction heated food often consider the geometric center of the can is the position of the cold spot despite presence of headspace which might not be correct as explained by [10]. Recently, Mohamed [10] developed a systematic procedure for determination of col spot for conduction heated canned food using an inverse heat conduction approach.

The well-known and established methods of thermal process calculations are either the formula method or the general method. Both of these methods use time-temperature data at the cold spot for calculating the required process time to achieve a targeted lethality level. The general method is based on integrating the lethal rate over both the heating and the cooling cycles utilizing either numerical or graphical techniques, while the formula method is based on calculating empirical heat penetration parameters from time-temperature data and then using various known formula methods. The techniques of thermal process calculations are presented in various published works [11-17]. The Time-temperature data at the cold spot can be obtained by either measuring temperatures at a predetermined time interval using thermocouples embedded at the geometric center of a can during retorting operation, or is based on using numerical solution to solve the heat transfer equation for canned food subjected to a given heating and cooling boundary conditions.

Numerical heat transfer models for predicting time-temperature at any position for packed food in containers are becoming more attractive recently due to the wide availability of high speed computers capable of providing very accurate prediction of time-temperature at the cold spot for various complex boundary conditions. Numerous published research works address the solution of the governing heat equation for various geometry and boundary conditions using different numerical methods. Teixeira, Dixon [18] were the first to develop a 2-D numerical computer

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model to simulate thermal processing of canned foods in cylindrical geometry using explicit finite difference method with the assumption of infinite surface heat transfer coefficient (negligible external surface resistance) for both heating and cooling cycles using constant retort temperatures. Other researchers followed Teixeira, Dixon [18] but allowing for variable retort temperature in order to optimize product quality during thermal processing [19, 20]. To overcome the assumption of negligible external thermal resistance which is not accurate during heating with air steam mixture, hot water heating, water cooling and at can headspace some researcher used finite thermal resistance at the boundary to improve prediction accuracy [21-25]. However, the challenge in using finite surface heat transfer coefficient in modeling and simulation of thermal sterilization processes rely greatly on the accuracy of the heat transfer coefficients and the numerical algorithm used. The explicit and implicit finite difference methods are very popular in modeling and simulation of thermal sterilization. However, the accuracy of both scheme rely on time step size used as the truncation errors decrease with decrease in step size. For the explicit method the stability considerations restrict the selection of the step size while such restriction is not of a concern with the implicit method. Therefore, in term of accuracy the implicit method is superior as it is unconditionally stable this will allow using small time step size which reduces truncation errors? On the other hand, some favor the explicit method due to it is simplicity and it requires less computer time. The second claim recently is not justifiable due to the availability of affordable high speed computers. Recently, greater attention were focused on using computational fluid dynamic (CFD) software to model thermal sterilization process for packaged foods in different geometries such as cans, glass jars and flexible packages [1, 6, 26]. Despite the sophistication of CFD algorithm and its capability of handling irregular geometries and multiphase food system but often simplified assumptions are used such as zero headspace and constant or variable temperature at the package boundary [1, 6, 26-28] such simplifications might not be accurate in representing the actual situation as can headspace is a reality and the boundary temperature is not the same as heating or cooling medium temperature due to existence of thermal boundary layer. Expressing the boundary conditions in term of heat transfer coefficients will be more realistic, therefore the objectives of this research are: 1) to develop a generalized computer simulation model that uses convective boundary conditions to handle finite and infinite external thermal resistance and account for the thermal resistance at the can headspace 2) to validate the model using published experimental data and to locate the cold spot.

MATHEMATICAL MODEL AND SIMULATION

Heat Transfer Model

For conduction heating and cooling in cylindrical can the governing differential equation is given by the following Fourier's equation:

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial^2 r} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial^2 z}\right) \quad (1)$$

Subjected to the following initial and boundary conditions:

Initial conditions:

$t = 0$, $T = T_o(0,r,z)$

Boundary conditions:

at $r = R$, z = 0 $\quad -k\frac{\partial T}{\partial r} = h_R(T_{SR} - T_R)$

at $z = L$ $\quad -k\frac{\partial T}{\partial z} = h_L(T_{SL} - T_R)$

Symmetry condition:

at $r = 0$ $\quad -k\frac{\partial T}{\partial r} = 0$

where, h_R represents the heat transfer coefficient at the can surface in the radial direction and at the bottom of the can and h_L represents the heat transfer coefficients at the can headspace side. During the cooling cycle h_R will be updated for the value that corresponds to the cooling medium condition.

Numerical Solution

Mohamed [8] developed a computer program written in FORTRAN language using an alternating direction implicit (ADI) finite difference method based on Crank-Nicolson scheme for solving Eq. (1) subjected to constant initial temperature and infinite surface heat transfer coefficient. In the current study the previously developed computer program was modified to account for both finite and negligible external thermal resistance by expressing the boundary conditions in term of heat transfer coefficients. The program also allows for use of different values of heat transfer coefficients at any given time in addition of updating the heat transfer coefficient when going from heating to cooling or during cooling. Different values of both space and time step sizes can be used due to the flexibility of the implicit scheme used. However, the number of nodes used in this study is 20 in both radial and axial direction and the time step used is one second.

Computer Program Validation

The computer program was validated using published experimental heat penetration data for 5% (w/w) bentonite in cylindrical can with diameter and height (98x110 mm) and headspace of 10 mm. Six cans with thermocouples embedded at their geometric center were processed in still retort for 104 min using saturated steam followed by water cooling [29]. The input to the computer program includes thermal properties data mainly thermal diffusivity and thermal conductivity which were determined as described by Mohamed [8]. A heat transfer coefficient of 800,000 W/(m^2- ^oC) was used during the heating cycle and this represent negligible external thermal resistance due to the use of condensing steam. At the headspace side a heat transfer coefficient of 54 W/(m^2- ^oC) suggested by Mohamed [30] was used during both the heating and cooling cycles. The protocol used during cooling was not explained in the paper by Teixeira, Balaban [29]. However, Tucker and Clark [4] suggested that during the first three minutes of the cooling phase, the heat transfer coefficient will be extremely high and can be taken as an infinite, for the rest of the cooling cycle they suggest a heat transfer coefficient of 600 W/(m^2-^oC). This protocol was adopted for this study for simulating the cooling phase. During execution of the program it is required to provide the value of the retort temperature at each time step which is selected to be one second in this study. However, the experimental retort temperatures were recorded at a discrete interval of one minute. In order to provide values for the retort temperature at any time, the retort temperature must be represented by continuous functions. For this reason the retort experimental time-temperature data were segmented into three phases; the first phase is the come-up time, during this phase the retort temperatures were assumed to be linear with respect to time, the second phase is the processing time, during this phase a constant retort temperature of (121 ^oC) was used and the third is the cooling phase, during this phase the entire retort temperatures were fitted to a logistic model.

RESULTS AND DISCUSSION

The entire measured retort temperatures during cooling were fitted to a logistic model using Sigma plot software. The model resulted in an excellent fit to the experimental time-temperature data (R^2 = 0.999) and the standard error (0.5363), yielding the following equation:

$$TR(t) = 19.6294 + \frac{101.9347}{[1+\left(\frac{t}{3.6463}\right)^{0.9764}]} \quad (2)$$

Figure **1** shows predicted retort temperatures, measured retort temperatures and predicted can center temperature as a function of time. It is quite obvious that the models used for expressing the retort temperatures as continuous functions for both the heating and cooling cycles were appropriate. The predicted can center temperature showed an inertia effect, which is a continuous increase in the center temperature for few minutes following commencement of cooling. Such trend is typically found in experimental heat penetration tests for food materials; such trend was attributed to the low thermal conductivity of food materials resulting in delayed response of the center to changes at the external can surface. Figure **2** shows predicted and experimental can center time-temperature data along with the experimental retort temperature profile. It is quite clear that predicted can center temperature follow exactly the response of the experimental data indicating the accuracy of the model. Expressing the boundary conditions in term of heat transfer coefficient provide great robustness to the current model as negligible external thermal resistance which is the case when heating is by condensing steam was handled very well by assigning very high value for the heat transfer coefficient during the heating phase. Also, the finite value of the heat transfer coefficient used for the can headspace proof to be accurate due to the overall accurate prediction during the heating phase. The contribution of the heat transfer from the can bottom and top for the can used in this study is compared to that from the side because the ratio of the height to diameter is 1.1. This indicates that the contribution from the headspace side is appreciable which demonstrates that the use of finite thermal resistance for the headspace side is an appropriate treatment. The recommended protocol of [4] used to for the cooling phase seem to work quite well as the model prediction of the can center temperature follow the response of the experimental can center temperature during this phase. After three minutes from the commencement of the cooling the heat transfer coefficient was updated to the value of 600 W/(m^2- ^{o}C), during this period only finite values of heat transfer coefficients were used, one at the can side normal to the radial direction and at the bottom of the can the other is at the can headspace side. This shows the capability of the model in using different values of heat transfer coefficients at any given time in addition of continuous updating the values of the heat transfer coefficient during the progress of the thermal sterilization process. A subroutine was incorporated into the program to calculate the thermal process lethality (F-value) using predicted can geometric center temperature by numerically integrating the following equation using Simpson's Rule:

$$F = \int_0^t 10^{\frac{T-TR}{z}} \qquad (3)$$

where T_R is a reference temperature (T_R = 121) and Z = 10^{o}C. The computed F-value for both heating and cooling phase based on numerical simulation is 6.72 (min),

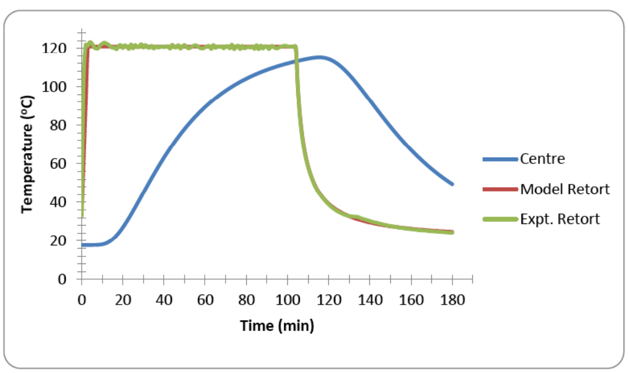

Figure 1: Model retort temperature, experimental retort temperature and predicted can center temperature as a function of time (experimental data from Teixeira *et al*. 1999).

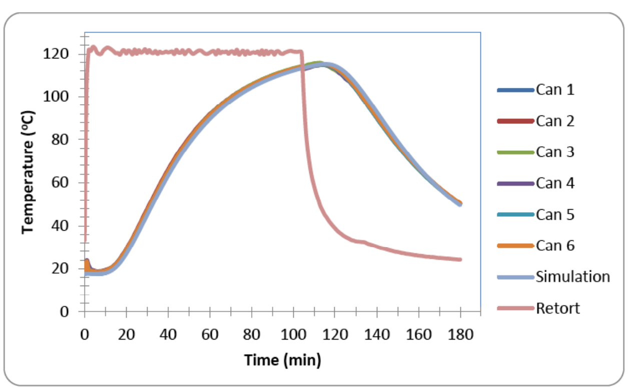

Figure 2: Simulation and experimental can center temperature versus time (experimental data from Teixeira *et al*. 1999).

while the F-vale based on the experimental heat penetration data for the six cans ranges between 6 to 7 minutes [29]. It is clear that the F-value from the computer simulation model is within the range of the experimental value which confirms the accuracy of the computer model in predicting can center temperature. It also worth to mention that the computer program could be easily modified to calculate thermal process lethality at any position within the can, this will help in calculating the integrated lethality that takes into consideration the variations of the temperature distribution within the can. It is also possible to evaluate product quality changes at any position within the can if the kinetic data for product quality component is known. The excellent results obtained from the computer simulation model indicates that considering actual heat transfer coefficient at the can headspace and considering finite thermal resistance during the cooling is more realistic situation. However, the actual position of the cold spot in presence of headspace need to be confirm in order to precisely evaluate the thermal process lethality. With model such as the current one which takes into consideration finite resistance at the can headspace it is readily straightforward to solve for the temperature distribution at any time along the axial central axes. This will allow for locating the cold spot to illustrate this point, the temperature profile along the axial central axes is calculated at selected time of 3600 second. Figure **3** shows the axial temperatures profile along the central axis, the bottom of the can is at node zero and the headspace at node 20. The figure clearly shows that the temperature profile is ax-symmetric which is obviously as anticipated since the heat transfer at the bottom is infinite while at the headspace side is finite.

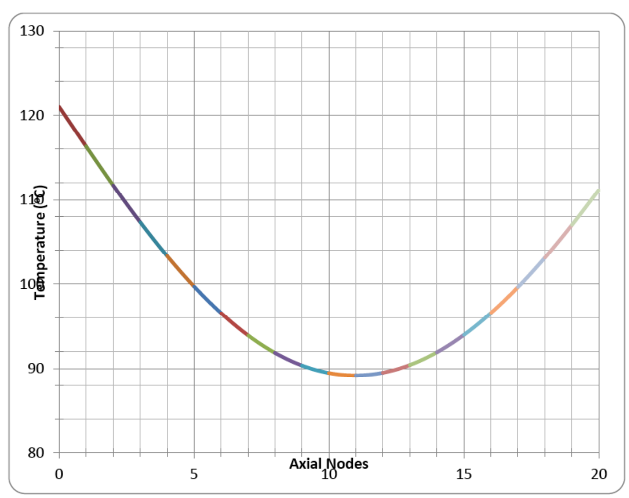

Figure 3: Axial central axis temperature profile at time 3600 second.

From the plot the cold spot is located at node 11 which correspond to a length value of 550 mm from the bottom of the can which incidentally confirm that for these particular cans and with the level of the headspace used the cold spot is at the geometric center. These clearly demonstrate the capabilities of the developed computer simulation models in enhancing thermal process design, in optimizing food product quality and assuring the safety of the canned foods in an efficient and inexpensive manner.

CONCLUSIONS

An implicit finite difference computer model based on the numerical solution of a two dimensional heat equation in cylindrical can geometry with the boundary conditions expressed in term of heat transfer coefficients was developed. The performance of the computer simulation for predicting the time-temperature profile at the geometric center was tested by comparison with experimentally determined time-temperature profile from the literature. The predicted time-temperature profile closely follows the experimental time-temperature profile during both heating and cooling phases in addition; the calculated F-value is within the range of the experimental value. The program was used successfully to locate the cold spot by examining the solution of the temperature profile along the central axis.

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NOMENCLATURE

h_L= heat transfer coefficient at the can headspace side W/(m^2 - ^{o}C)

h_R= heat transfer coefficient at the can side and bottom W/(m^2 - ^{o}C)

k= thermal conductivity, W/(m - ^{o}C)

L= height of the model food, mm

r= radial cordinate, mm

R= radius of the can, mm

t= time, s

T= temperature, ^{o}C

T_o= initial temperature, ^{o}C

T_R= retort temperature, ^{o}C

T_{SR}= temperature at the surface normal to the radial direction and at the bottom, ^{o}C

T_{SL}= surface temperature at the headspace side, ^{o}C

z= axial coordinate, mm

Z= slope index of the thermal death time curve of a target microorganism, ^{o}C

GREEK

α= thermal diffusivity m^2/s

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