Thermophysical Property Influence in Model Accuracy for the Sterilization Process

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Abstract: - To know the accurate value of a thermophysical property is an important factor in the prediction ability of any proposed model for heat transfer. In this work, the influence of the thermophysical property accuracy in the mathematical model predictions for a sterilization process is studied. A simulation was done using the finite difference method with the implicit direction alternating (IDA) solution scheme. Thermophysical property variations (\pm 25%) were done and it was observed their influence in the process design variable values obtained with the mathematical model proposed. For perturbations below 10%, results showed a linear relationship between variation in the thermophysical property values and in the predicted sterilization time. When the perturbation percentage was over 10%, the predicted sterilization time variation increases in a percentage bigger than the perturbation one.

Key-Words- Thermophysical property, simulation, numerical modeling, finite difference, sterilization.

1 Introduction

In recent years, computer simulations have shown to be a valuable tool to predict the food processing and storing conditions [1], leading to money and time savings in the design and sizing of equipments. When a mathematical model is developed, the selection of the most convenient numerical approach (finite difference, finite element and finite volume) has become of extreme importance [2].

Because of the mathematical model usefulness, a big effort has been done to increase its accuracy by improvement of the quality of data like heat and mass transfer areas, transfer coefficients, volume changes and food properties [2]. In the other hand, new simulation tools like the artificial neural networks [3] can generate enough accurate model results without exact values of those variables. Another alternative for improving the model accuracy is to simulate coupled phenomena, for example mass and heat transfer in food processing [4,5].

It is difficult to determine the value of the thermophysical properties for a food, because of its particular characteristics like irregular shapes, changing compositions and anisotropic properties. When some of those variables are used in a mathematical model, it is possible to use not entirely accurate values. In the specific case of food properties needed for heat transfer modeling, their values can be as different as the sources for obtaining them.

Fricke and Becker [6] determined the influence of the heat transfer coefficient in the calculated cooling time for different models. They found that for the most of the studied models, deviation of 20% in heat transfer coefficient, produced deviation of 5% in the predicted cooling time.

Thermophysical properties can be determined by complicated experimental procedures [7-11] or by a simple expression evaluation [12-15]. In any case, the method to be selected will depend on a balance between availability and exactness of the required property.

Because not always it is possible to get the exact thermophysical property values, it is important to know how their variations can affect the process variable value predicted by a heat transfer mathematical model. That is the objective of this work.

2 Problem Formulations

The sterilization process proposed by Mohamed [16] is a representative model of a heat transfer process in food industry. The purpose of the model is the prediction of temperature history inside a can. This problem can be represented by a cylindrical coordinates system (Fig.1).



Fig. 1. Cylindrical coordinates system.

The energy balance in cylindrical coordinates can be written with equation (1).

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

Initial Condition

$$T(r,z,0) = T_0 \qquad 0 \le r \le R \qquad 0 \le z \le H$$

Boundary conditions

$T(R,z,t) = T_b$	$0 \le z \le H$	t>0
$T(r,H,t) = T_b$	$0 \le r \le R$	t>0
$T(r,0,t) = T_{\rm b}$	$0 \le r \le R$	t>0

These conditions are variable in time, because in the real process the can is suddenly exposed to a high temperature and later it is cooled down to the initial temperature (Fig. 2).



Fig. 2. Sterilization process conditions

Additionally, at the center of the can there is a condition of symmetry:

$$\frac{\partial T}{\partial x}(0,z,t) = 0 \quad 0 \le z \le H \quad t > 0$$

For process design, it is desired to determine how long must be the can at the heating temperature, to assure that all its points reach the required sterilization temperature. The critical point in the can is its center, because it is far away the can borders and it has a temperature variation rate slower than the external points.

In a process like sterilization, the high temperature exposure time must be controlled to avoid food damage or unnecessary energy expenses.

3 Problem Solutions 3.1 Numerical Scheme

To solve equation (1), the finite difference method with the implicit direction alternating (IDA) solution scheme was used [17]. This method has two advantages: The convergence of an implicit method and the saving in time calculation associated with the use of tridiagonal matrices.

The system was divided in a square mesh with sides $\Delta r=R/n$ and $\Delta z=H/m$ (Fig. 3). The modeled cylinder is R=3 cm radius and H=4.07 cm height. Discretized spatial variables are: $r=i\Delta r$ and $z=j\Delta z$. Discretized temperature is in equation (2).

$$T(r, z, t) = T_{i, i}^{k}$$
⁽²⁾

where, i=1,2,3...n-1 and j=1,2,3...m-1



Fig. 3. Cylindrical coordinates discretization

3.1.1 First iteration: Implicit in r

Terms which are multiplying the temperature values are grouped in a matrix, eq. (3).

$$M1(i) = \begin{pmatrix} -\frac{\alpha\Delta t}{\Delta r^{2}} \left(1 - \frac{1}{2i}\right) & \frac{\alpha\Delta t}{\Delta z^{2}} \\ 1 + \frac{2\alpha\Delta t}{\Delta r^{2}} & 1 - \frac{2\alpha\Delta t}{\Delta z^{2}} \\ -\frac{\alpha\Delta t}{\Delta r^{2}} \left(1 + \frac{1}{2i}\right) & \frac{\alpha\Delta t}{\Delta z^{2}} \end{pmatrix}$$
(3)

Because IDA is used, tridiagonal systems are obtained (A' matrix). The elements of the three main diagonals of the matrix A' are stored in a not square matrix (n-1x3), eq. (4).

$$A = \begin{pmatrix} 0 & Ml(1)_{1,1} + Ml(1)_{2,1} & Ml(1)_{3,1} \\ Ml(2)_{1,1} & Ml(2)_{2,1} & Ml(2)_{3,1} \\ Ml(3)_{1,1} & Ml(3)_{2,1} & Ml(3)_{3,1} \\ \vdots & \vdots & \vdots \\ Ml(n-1)_{1,1} & Ml(n-1)_{2,1} & 0 \end{pmatrix}$$
(4)

The vector of independent terms is shown in equation (5).

For j = 1, 2, 3...(m-1)

$$Ab(j)^{k-1} = \begin{pmatrix} \sum_{f=1}^{3} Ml(1)_{f,2} T_{l,j+f-2}^{k-1} \\ \sum_{f=1}^{3} Ml(1)_{f,2} T_{2,j+f-2}^{k-1} \\ \sum_{f=1}^{3} Ml(1)_{f,2} T_{3,j+f-2}^{k-1} \\ \vdots \\ \sum_{f=1}^{3} Ml(1)_{f,2} T_{n-1,j+f-2}^{k-1} - Ml(1)_{3,1} T_{b} \end{pmatrix}$$
(5)

For each value of "j", a linear system of (n-1) equations is solved by equation (6).

$$A'.T_{i,j}^{k} = Ab(j)^{k-1}$$
(6)

Since A' is a tridiagonal matrix, the system can be solved by Thomas' algorithm [18].

3.1.2 Second iteration: Implicit in z

In a similar way as for the spatial variable "r", the system matrices were defined, (eqs. 7, 8, 9)

$$M2(i) = \begin{pmatrix} -\frac{\alpha\Delta t}{\Delta z^2} & \frac{\alpha\Delta t}{\Delta r^2} \left(1 - \frac{1}{2i}\right) \\ 1 + \frac{2\alpha\Delta t}{\Delta z^2} & 1 - \frac{2\alpha\Delta t}{\Delta r^2} \\ -\frac{\alpha\Delta t}{\Delta z^2} & \frac{\alpha\Delta t}{\Delta r^2} \left(1 + \frac{1}{2i}\right) \end{pmatrix}$$
(7)

$$B = \begin{pmatrix} 0 & M2(1)_{1,1} & M2(1)_{2,1} \\ M2(1)_{1,1} & M2(1)_{2,1} & M2(1)_{3,1} \\ M2(1)_{1,1} & M2(1)_{2,1} & M2(1)_{3,1} \\ \vdots & \vdots & \vdots \\ M2(1)_{1,1} & M2(1)_{2,1} & 0 \end{pmatrix}$$
(8)

For i=1, 2, 3...(n-1)

$$bb(i)^{k} = \begin{pmatrix} \sum_{f=1}^{3} M2(i)_{f,2} T_{i+f-2,1}^{k} - M2(i)_{1,1} T_{b} \\ \sum_{f=1}^{3} M2(i)_{f,2} T_{i+f-2,2}^{k} \\ \sum_{f=1}^{3} M2(i)_{f,2} T_{i+f-2,3}^{k} \\ \vdots \\ \sum_{f=1}^{3} M2(i)_{f,2} T_{i+f-2,m-1}^{k} - M2(i)_{3,1} T_{b} \end{pmatrix}$$
(9)

In this case, for each "i", a linear system of (m-1) equations is solved by eq. 10.

$$\mathbf{B}'.\mathbf{T}_{i,i}^{k+1} = \mathbf{b}\mathbf{b}^k \tag{10}$$

3.2 Thermophysical Properties

Thermal diffusivity (α) values were obtained from Azoubel *et al.* [19] for Cashew juice, which are calculated with the equation (11).

$$\alpha = 1.45751 \times 10^{-7} - 0.00558 \times 10^{-7} \text{C}$$
(11)

where C is concentration in °Brix, α in m²s⁻¹.

3.3 Temperature History

The model was solved for a 10x10 mesh, because there is no variation in the results with this step size. The results of the temperature at the center of the can are shown in figure 4, for cashew juice, 30 °Brix. Thermal diffusivity obtained by equation (11) is α =1.29x10⁻⁷ m²s⁻¹.



Fig. 4. Temperature history at the center of the can.

The results show that the center of the can reaches the desired temperature of 120 °C in approximately 79 minutes.

The thermal diffusivity value is modified in \pm 15%. The temperature at the center is shown in Fig. 5, for α values between 85 and 115% of the initial value.



Fig. 5. Temperature (center of the can) at different α values.

It can be observed how the temperature history inside the can is strongly affected by changes in thermal diffusivity values. Higher values of α predict faster temperature changes. Lower values of α predict slower temperature changes

3.4 Heating Time

Heating time percentage absolute deviation is shown in Fig. 6, for α values between 75 and 125

% of the initial value. Value of α of 75% initial value (25% down deviation) produces an absolute deviation of 33% in the predicted heating time. A 25% α upper deviation produces an absolute deviation of 20% in the predicted heating time. When absolute α deviations are below 10%, the absolute deviations on the model result are almost 1:1.



Fig. 6. Heating time deviation vs. α variation

Depending on the type of deviation, the consequence over the food is different. If the food is heated more time that it is necessary, this condition can cause damage by thermal degeneration. In the other hand, if the food is heated less time that it is necessary, some regions in the food can not reach the sterilization temperature and the micro-organisms won't be totally eliminated.

At first sight, the variations in thermal diffusivity may be considered too high, but it has to be taken into account the anisotropic nature of foods and their properties related to the heat transfer. Moreover, foods are basically constituted by water, which can change in 20% its thermal diffusivity value when temperature rises from 20 to 100 °C [8]. For this reason, the use of a unique α value in a mathematical model like this, can lead to an important error because of the big changes in the temperature. This error together with the deviations associated to the numerical method can contribute to get not accurate model predictions.

4 Conclusions

Influence of the exactness of a thermophysical property on the model prediction accuracy was determined. Absolute α deviations below 10% produce absolute deviations on the model prediction of similar magnitude. For sterilization process, it would be better to use variable thermal

diffusivity because of the sudden temperature changes, in order to improve model prediction.

Acknowledgement

The authors want to thank Decanato de Investigaciones y Desarrollo for its financial support and Professor Andrés Vidal for his valuable comments and suggestions.

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