Can Tho University Journal of Science
website: sj.ctu.edu.vn

DATA-BASED MECHANISTIC MODELING APPROACH FOR PREDICTING THERMAL RESPONSE OF CONDUCTIVE FOOD DURING HEATING PROCESSES

Nguyen Trung Truc[1], To Quang Truong[2], Le Thi Hoa Xuan[3] and Vo Tan Thanh[4]

[1]*Vinh Long University of Technology Education, Vietnam*
[2]*National Agro-Forestry-Fisheries Quality Assurance Department (zone 5)*
[3]*Dong thap Community College, Vietnam*
[4]*Department of Food Technology, Can Tho University, Vietnam*

ARTICLE INFO

Received date: 29/07/2015
Accepted date: 19/02/2016

KEYWORDS

Thermal processing, heat transfer coefficient, modeling

ABSTRACT

The application of data based mechanistic modeling approach to predict thermal histories of conductive foodstuffs during heating is reported. In the experiment, minced fish was filled in 307x113 steel cans as the conductive food. Step increase in heating medium was applied while the product temperature was recorded. The simplified refined instrumental variable algorithm was used as model parameter identification tool to obtain the best model order and parameters. As a result, the first order transfer function model is proved to be sufficiently enough for describing the heat transfer from heating medium to product with a high statistical significance (R^2 > 0.99). In this model, a parameter related to the heat transfer coefficient was found and could be used to predict the product temperature during heating processes.

Cited as: Truc, N.T., Truong, T.Q., Xuan, L.T.H., and Thanh, V.T., 2016. Data-based mechanistic modeling approach for predicting thermal response of conductive food during heating processes. Can Tho University Journal of Science. Vol 2: 63-68.

1 INTRODUCTION

Thermal processing is one of the major preservation technologies used for producing safe and shelf-stable food (Chen and Ramaswamy, 2004). Temperature, which is the most important process variable in most operations involving the transformation and preservation of foods, has a direct influence on the kinetics of chemical reactions, on enzymatic and microbial activities, etc. and it should be control during the processes.

Thermal processes calculations referred to the design and/or the evaluations of a thermal process are mainly dependent on the internal temperature changes with time of heating, and are broadly divided into two classes: "general method" and "formula methods". The "general method" integrate the lethal effects by a graphical or numerical integration procedure based on the time-temperature data obtained from test containers processed under actual commercial processing conditions during "formula methods" make use of parameters obtained from these heat penetration data together with several mathematical procedures to integrate the lethal effects (Hosahalli and Singh, 1997). In "formula methods", predicted product temperature is associated with constant retort temperature (Stoforos, 2010).

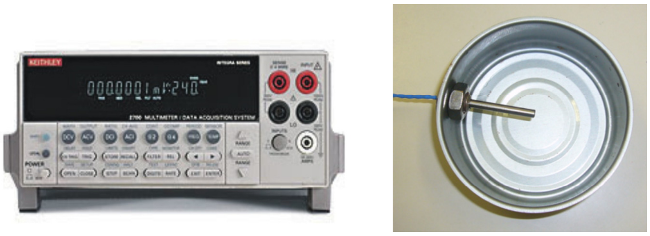
Most studies have only focused on the finding of the best fitting of transfer function in thermal processing (*black box model*), *i.e.* the black box modeling (Glavina *et al.*, 2006; Ansorena and Scala, 2009; Ansorena *et al.*, 2010). However, there is still a need for finding a physically meaningful parameter in a transfer function to predict and control product temperature during heating.

The objective of this work is to characterize the thermal response of canned conductive food in batch retorts and try to model the process by using a data-based mechanistic modeling approach.

2 MATERIALS AND METHODS

2.1 Laboratory test equipment

In this experiment, minced fish was filled in 307x113 steel cans as the conductive food. To obtain the temperature profiles, the calibrated type T thermocouples are positioned in the center of cans as Figure 1 and all thermocouples were connected to a digital data logger (Keithley 2700, USA).



(a) (b)

Fig. 1: (a) Analog Keithley 2700; (b) Sensor position

During thermal treatment, the container was placed in a water bath. The product and water temperature during experiment are recorded at 10-second interval.

To obtain the data sets for dynamic modeling, the steps up of temperature was adjusted from 50 to 80^{o}C, heating medium and product temperature were monitored for 160 minutes as Figure 2.

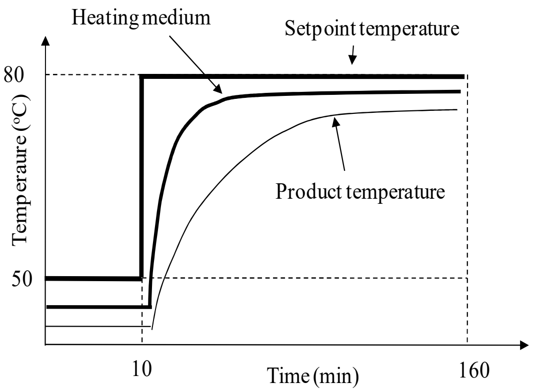


Fig. 2: Step up experiment

2.2 Data-based mechanistic (DBM) modeling approach

The term "data-based mechanistic modeling" was first introduced by Young and Lees in 1992 (cited in Young, 2002). This modeling approach obtained initially from the analysis of observational time-series but was only considered credible if it can be interpreted in the physically meaningful terms. As illustrated in Figure 3, the DBM approach consists of data based and mechanistic phases. The first step in DBM modeling is to identify a suitable mathematical model from a generic model class that is both capable of explaining the data in a parametrically efficient manner and having minimal complexity in terms of model order and model parameters. After this initial black-box modeling stage is complete, the model is interpreted in a physically meaningful, mechanistic manner based on the nature of the system under study and the physical, chemical, biological or socio-economic laws that are most likely to control its behavior.

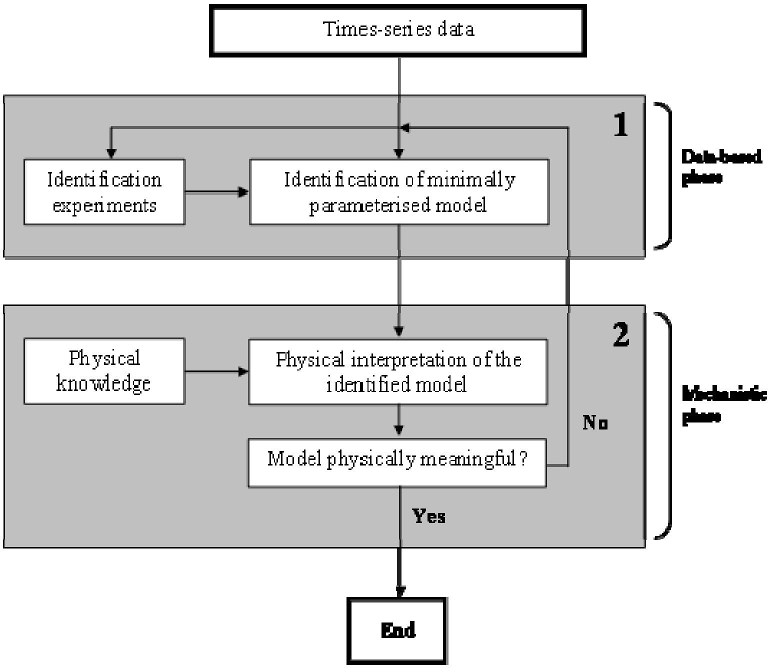


Fig. 3: Data based mechanistic (DBM) modeling technique

A continuous-time transfer function model for a single-input single-output (SISO) system has the following general form:

$$x(t) = \frac{B(s)}{A(s)} u\left(t - \tau\right) \text{ and } y(t) = x(t) + e(t) \text{ or}$$

$$y(t) = \frac{B(s)}{A(s)} u(t - \tau) + e(t)$$

Where A(s) and B(s) are the following polynomials in the derivative operator $s = \frac{d}{dt}$

$$A(s) = s^n + a_1 s^{n-1} + \ldots + a_{n-1} s + a_n$$

$$B(s) = b_0 s^m + b_1 s^{m-1} + \ldots + b_{m-1} s + b_m$$

2.2.1 Data phase in thermal processing

High frequent data (*10-second interval*) was obtained from dynamic experiments. In the "Data-based phase", a dynamic transfer function model was fitted through data and evaluated on its accuracy. Although other techniques are available, in this study the simplified refined instrumental variable (SRIV) approach was used as a method for model identification, since it not only yields consistent estimates of the parameters but also exhibits close to optimum performance in the model order reduction context (Young, 1984).

The ability to estimate the parameters represents only one side of the model identification problem. Equally important is the problem of objective model order identification resulting in low complexity. The process of model order identification can be assisted by the use of well-chosen mathematical measures which indicate the presence of over parameterization. A reasonably successful identification procedure used to select the most appropriate model structure is based on the minimization of the young identification criterion, YIC (Young *et al.*, 1981). The Young Identification Criterion (YIC) is a heuristic statistical criterion, which consists of three elements. The first term provides a normalized measure of how well the model explains the data: the smaller the variance of the model residuals in relation to the variance of the measured output, the more negative this term becomes. The second term is a normalized measure of how well the model parameter estimates are defined for the order model, the smaller the relative error variance, the better defined are the parameter estimate in statistic terms, and this is one more reflected in a more negative value for the term. The third term provides a compromise between goodness of fit and number of parameters, model order increased, so the first term tends to decrease, while the second term tends to decrease at first and then to increase quite markedly when the model becomes over parameterized and the standard error on this parameter estimates becomes larger in relation to the estimated values.

Consequently, the model, which minimizes the YIC, provides a good compromise between goodness of fit and parametric efficiency. While the YIC ensures that the model is not over parameterized, it is not always good at discriminating models that have a lower order than the 'best' model. Because of this, the YIC will often, if applied strictly, identify a model that is under-parameterized. Therefore, it is used together with the coefficient of determination R^2. If the YIC identified model has an adequate R^2, which is not significantly lower than the R^2 of the higher order models, it may be fully accepted as the best model in identification terms.

2.2.2 Mechanistic phase in thermal processing

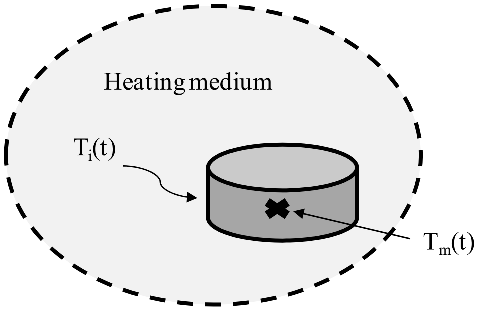


Fig. 4: Heat transfer during heat treatment

Assuming uniformity of product temperature during heat treatment, the heat transfer between heating medium to product as shown in Figure 4 is governed by the following equation:

$$m.C_{\mathrm{p,m}} \frac{\mathrm{d}T_{\mathrm{m}}(t)}{\mathrm{d}t} = k_{\mathrm{m}}.S_{\mathrm{m}}(T_{\mathrm{i}}(t) - T_{\mathrm{m}}(t)) \qquad (1)$$

Where m: mass of product (kg); $C_{p,m}$: specific heat of product (J/kg °C); k_m: heat transfer coefficient (W/m^2 °C); S_m: surface of product (m^2); $T_i(t)$: heating medium temperature at time (°C); $T_m(t)$: product temperature at time (°C).

The **Eq. 1** can be rewritten as:

$$\frac{\mathrm{d}T_{\mathrm{m}}(t)}{\mathrm{d}t} = \frac{k_{\mathrm{m}}.S_{\mathrm{m}}}{m.C_{\mathrm{p,m}}}(T_{\mathrm{i}}(t) - T_{\mathrm{m}}(t)) \qquad (2)$$

Let

$$\alpha = \frac{k_{\mathrm{m}}.S_{\mathrm{m}}}{m.C_{\mathrm{p,m}}} \qquad (3)$$

Where α is a heat transfer rate (1/s)

The **Eq. (2)** can be written as:

$$\frac{\mathrm{d}T_{\mathrm{m}}(t)}{\mathrm{d}t} = \alpha(T_{\mathrm{i}}(t) - T_{\mathrm{m}}(t)) \qquad (4)$$

Under steady state condition $\left(\frac{dT_m}{dt} = 0\right)$, and **Eq. (4)** will become

$$\alpha(\bar{T}_{\mathrm{i}} - \bar{T}_{\mathrm{m}}) = 0 \qquad (5)$$

If we only consider small temperature perturbations ($t_i(t)$, $t_m(t)$) around steady state, subtracting **Eq. (5)** from **Eq. (4)** results in:

$$\frac{\mathrm{d}t_{\mathrm{m}}(t)}{\mathrm{d}t} = \alpha(t_{\mathrm{i}}(t) - t_{\mathrm{m}}(t)) \qquad (6)$$

After converting **Eq. (6)** with the Laplace operator, the transfer function results in:

$$t_{\mathrm{m}}(t) = \frac{\alpha}{s+\alpha} t_{\mathrm{i}}(t) \qquad (7)$$

The α value in **Eq. 3** contains an important parameter; it is a heat transfer coefficient k_m which is related to medium characteristics, medium velocity and surface of product.

3 RESULTS AND DISCUSSION

3.1 Change of heating medium and product temperature

Heating medium and product temperature were recorded and performed in Figure 5. Product temperature was reached to medium temperature after 100 min.

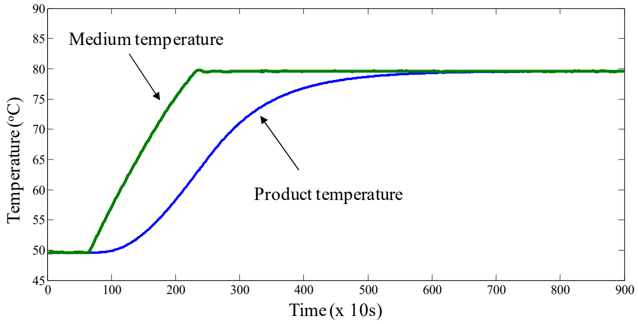


Fig. 5: Heating medium and product temperature during experiment

3.2 Data-based phase in heating process

Applying continuous-time simplified refined instrumental variable (SRIV) algorithm (Young, 1981) to estimate the parameters in the first and second order transfer function, based on coefficient of determination R^2 and minimization of the YIC value in the test as the example of for the calculating method.

Table 1: The model parameter estimates for heating process

TF	[m, n, τ]	Model parameters	SE	R^2	YIC
First order	[0, 1, 28]	a_1= 0.0105 b_0= 0.0106	0.0077	0.9999	-23.15
Second order	[1, 2, 28]	a_1= 0.0191 a_2= 0.0001 b_0= 0.0104 b_1= 0.0001	0.0057	0.999	-12.52

TF: transfer function; SE: standard error of equations; R^2: coefficient of determination; YIC: Young identification criterion; m, n and τ, denominator, numerator and time delay; a_1, a_2, b_0, b_1, parameters in the first and second order of transfer function

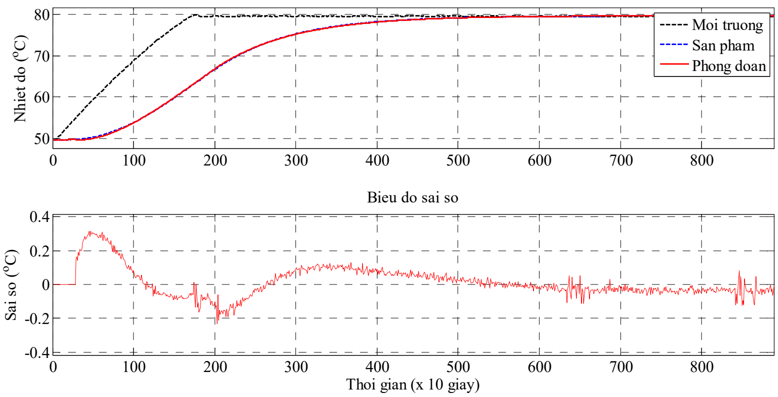


Fig. 6: The output of the first order of transfer function model compared with the measured temperature response (above) and residual plot (below)

From Table 1, it is obvious that the first and the second order transfer function can be applied. The second order of transfer function is the best fitting model, but the first order has a lower value for YIC and will be selected as the best fitted model. The first order of transfer function model compared with the measured temperature response and the residual plot are shown in Figure 6.

The selected model from this experiment in form:

$$t_m(t) = \frac{0.0105}{s+0.0106} t_i(t-\tau) \qquad (8)$$

3.3 Physical meaningful parameter in a model

The second step in data-based mechanistic modeling approach is interpreted in a physically meaningful way based on the nature of the system (Young and Garnier, 2006). In this research, the first order of fitted model was selected to seek the physical meaning of this process. From Eq. (7) and (8), the importantly found value α is equal to b_0, was defined as a "heating rate" term in relation to heat transfer coefficient from the heating medium to product and the estimated parameters a_1 and b_0 are not very different, also proved the accuracy of selected model.

3.4 Applying of a selected model for predicting of product temperature during heat treatment

The transfer function performed in **Eq. 8** contained a physically meaning parameter. So, it is possible to apply to predict product temperature during heat treatment and can be used to online calculate F-value (*Least Sterilizing Value*) during heat treatment.

The algorithm to predict product temperature was presented in Figure 7.

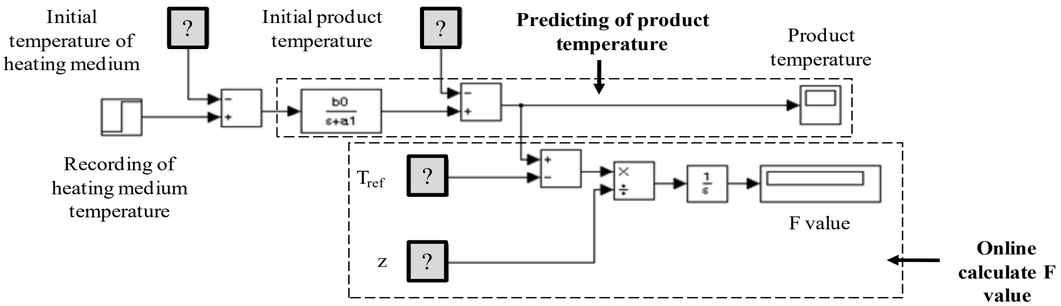


Fig. 7: The algorithm to predict product temperature during heating

From **Figure 7,** with initial of product temperature, initial temperature of heating medium and recording heating medium, the predicting product temperature can be obtained. It is a basic for online calculating of the F-value with temperature reference (T_{ref}) and thermal resistance (z).

4 CONCLUSIONS

The application of data-based mechanistic modeling approach to predict thermal histories of conductive foodstuffs when surroundings present different forcing functions during heating of processes was reported in this paper. The comparison of experimental data with proposed model presented a very satisfactory result with the first-order transfer function. A physically meaningful parameter found in this model is a heat transfer coefficient from heating medium to product, which can be used to predict and control a product temperature during heating process.

REFERENCES

Ansorena, M.R., Di Scala, K.C., 2009. Predicting Thermal Response of Conductive Foods during Start-up of Process Equipment Using Transfer Function. Journal of Food Process Engineering. 33: 168–181.

Ansorena, M.R., del Valle, C.E., Salvadori, V.O., 2010. Application of Transfer Functions to Canned Tuna Fish Thermal Processing. Food Science and Technology International. 16(1): 43–51.

Chen, C.R., Ramaswamy, H.S., 2004. Multiple Ramp Variable Retort Temperature Control for Optimal Thermal Processing. Food and Bioproducts Processing. 82: 78-88.

Glavina, M.Y., Di Scala, K.C., Ansorena, R., del Valle, C.E., 2006. Estimation of thermal diffusivity of foods using transfer functions. LWT- Food Science & Technology. 39: 455-459.

Hosahalli, S.R., Singh, R.P., 1997. Chapter 2: Sterilization Process Engineering in Handbook of Food Engineering Practice. CRC Press.

Stoforos, N.G., 2010. Thermal Process Calculations through Ball's Original Formula Method: A Critical Presentation of the Method and Simplification of its Use through Regression Equations. Food Engineering Reviews. 2: 1–16.

Young, P.C. 1981. Parameter estimation for continuous-time models—a survey. Automatica. 17: 23–39.

Young, P.C., 1984. Recursive Estimation and Time-Series Analysis. Springer-Verslag, Berlin, Germany.

Young, P.C., 2002. Data-based mechanistic and top-down modelling. Proceedings of the First Biennial Meeting of the International Environmental Modelling and Software Society, iEMSs, Manno, Switzerland, ISBN:88-900787-0-7.

Young, P.C., Garnier, H., 2006. Identification and estimation of continuous-time, data-based mechanistic models for environmental systems. Environmental Modelling & Software 21: 1055–1072.