A NEURAL NETWORK APPROACH FOR THERMAL PROCESSING APPLICATIONS

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Accepted for Publication May 10, 1995

ABSTRACT

The use of a neural network approach in thermal processing applications is presented. A four layer neural network with 3 inputs and 3 outputs was trained using a back-propagation algorithm. A finite difference computer program was used to predict nodal temperature responses of conduction heating model foods under thermal processing conditions. Equivalent lethality processes were obtained for a range of input variables (can size, food thermal diffusivity and kinetic parameters of quality factors) for sterilization temperatures between 110 and 134C (at 2C intervals). The computed optimum conditions and their associated quality changes were used as input variables for training and evaluation of the neural network. The trained network was found to predict optimal sterilization temperatures with an accuracy of \pm 0.5C and other responses with less than 5% associated errors.

INTRODUCTION

Food industry is pressed with the need to provide foods that are safe, nutritious and convenient at competitive prices. In the last decade, various studies have been carried out for quality optimization of thermally processed foods. Computer simulation has made this possible since kinetics of microorganisms and quality factors, and physics of conduction heat transfer are very well understood and can be described with mathematical models. Optimization of sterilization process is based on the fact that thermal inactivation of microorganisms is much more temperature dependent than quality factors (Lund 1977) and

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Journal of Food Processing and Preservation 19 (1995) 283-301. All Rights Reserved. [®]Copyright 1995 by Food & Nutrition Press, Inc., Trumbull, Connecticut. has lead to the use of high temperature short time (HTST) processing. However, applicability of this principle to conduction heated foods is limited due to their slow heating behavior resulting in large temperature gradients within the can during heating/cooling. Teixeira *et al.* (1969) were probably the first to use computer simulations for quality optimization. They used a finite difference solution to conduction heat transfer equation for cylindrical cans coupled with kinetic data on nutrient degradation. Recently, several researchers have used such models for predicting optimal conditions for thermal processing of foods (Teixeira *et al.* 1969; Saguy and Karel 1979; Ohlsson 1980; Thijssen and Kochen 1980; Silva *et al.* 1992; Hendrickx *et al.* 1989, 1993).

Hendrickx et al. (1989) used an empirical approach to calculate optimal temperatures for maximizing quality factors. Using traditional regression analysis, they developed empirical equations to relate optimal temperatures to various product properties (thermal diffusivity and z-value of quality factors), processing conditions (geometry and dimensions of the food, surface heat transfer coefficient, initial product temperature and retort come up time) and processing criteria (target F_a-value). Hendrickx et al. (1993) extended the correlations for more generalized conditions accounting for cooling lethality as well as retort come up time. The study, however, was limited to infinite shapes with one dimensional heat transfer. Silva et al. (1992) presented the correlations for optimal sterilization temperature for conduction heating foods with finite surface heat transfer coefficients. Previously mentioned work (Hendrickx et al. 1989, 1993; Silva et al. 1992) was based on optimizing the surface quality. An extensive review of modeling optimum processing conditions for sterilization was presented by Silva et al. (1993). Recently Silva et al. (1992) presented a comparative study between surface and volumetric average quality retention in thermo processed foods.

ARTIFICIAL NEURAL NETWORK

An artificial neural network is a collection of interconnecting computational elements which is simulated like neurons in biological systems. It is characterized by the network topology, neurons and learning rules. Artificial neural network has the capability of relating the input and output parameters without any prior knowledge of the relationship between them. A properly trained neural network can be used to simultaneously produce more than one output, unlike traditional models where one regression is required for each output. Recently, artificial neural networks have been used in those situations where no good physical models of the process were available and the number of output variables were more than one (Linko *et al.* 1992; Huang and Mujumdar 1993). Artificial neural network models were originally developed to mimic the function of human brain. Brain contains billions of nerve cells (neurons) highly interconnected through synapses. Each neuron processes information by receiving signals from other neurons via synapses and produce an output which is then transmitted to some other neurons. It is believed that the synaptic strength of junctions is altered when knowledge is stored in the brain. Consequently, a synapse can be considered as the basic memory unit of the brain.



Desired Response

FIG. 1. MODEL OF AN ARTIFICIAL NEURON

The artificial neural network used in this study is a computer program that consists of a collection of simple elements (neurons) that work together to solve the problem. An artificial neuron is modelled (Fig. 1) to receive (n) inputs, $X = [x_0, x_1, x_2, ..., x_n]$ and yield a desired output (d), through a process of learning. The components of the input vector are weighted by a set of coefficients, W ($w_0, w_1, w_2, ..., w_n$). The sum of the weighted input is then computed, producing an output, $S = X^M W$ (X input vectors from Mth layer). The weights are essentially continuous variables and can take negative as well as positive values. During the learning process, input vectors and desired response are presented to the network, and an algorithm automatically adjusts

the weights so that output responses to input vectors will be as close as possible to their respective desired response. A popular method for adapting the weights is the simple LMS (least mean square) algorithm (Widrow and Lehr 1993) which minimizes the sum of squares of the linear error over the learning set. The linear error (ϵ) is defined to be the difference between the desired response (d) and the output (S). However, when this model is applied to a multi-element neural network, the procedure for error calculation becomes more complicated (Widrow and Lehr 1993).

The more common structure of an artificial neural network is generally of multilayer design. A fully connected four layer network is illustrated in Fig. 2. During learning, the response of each output neuron in the network is compared with a corresponding desired response. Error signals associated with the output elements are computed and the information transmitted from one layer to the previous layer using a back-propogation algorithm (hence the name back-propogation network). This procedure is repeated over the entire learning set for a specified number of times (learning runs), chosen by trial and error. In the layer structure, the inputs are interconnected in an input layer, and the computed outputs are interconnected in the output layer (Fig. 2). In between these two layers, one or more hidden layers (as another variable for neural network) depending upon the applications, are interconnected. The number of input neurons correspond to the number of input variables, and the number of output neurons match the number of desired output variables. The number of neurons in the hidden layer is dependent on the application of the network. In principle, if sufficient number of these input/output combinations are used for learning/training of neural network, such a trained network should be able to predict the output for new inputs. These learning sets can be compiled from experimental data if available or, as in the present study, the needed data can be obtained from computer simulation.



Input Layer Hidden layers Output Layer FIG. 2. SCHEMATIC OF ARTIFICIAL NEURAL NETWORK USED IN THE PRESENT STUDY

The objective of this study was to evaluate the use of neural network in predicting optimal thermal processing conditions. In the present study, due to lack of experimental data for constructing/learning of the neural network, a finite difference computer simulation was used to generate needed data on optimal sterilization temperatures, associated process times and quality factor retention. Neural network models can also be applied to situations where exact mathematical description of the process is not available or when prevailing conditions result in deviations from predictable behavior. In fact, neural network applications will have a greater impact/application under these situations. Because of the use of computer simulation for data input, in this study, the potential of neural network application may seen less obvious; however, it should not be viewed as a limitation.

METHODOLOGY

Process Optimization

An optimal sterilization temperature is generally taken as the processing temperature that results in minimum volumetric heating of the food product while meeting the constraints of commercial sterility. Such a process can be expected to preserve the bulk of thermolabile quality factors. Exceptions exist to this rule; for example, when surface discoloration due to thermal treatment is the primary consideration, the optimization should be aimed at minimizing surface cook rather than product bulk. Parameters that determine the optimal sterilization temperature are numerous: can dimension, thermal diffusivity of food, kinetic parameter of nutrient (z), lethality to be achieved, cooling water temperature, initial temperature of food, retort come up time, convective heat transfer coefficient at the can outer surface, etc. To obtain optimal sterilization temperatures in this study a mathematical model for conduction heat transfer in a cylindrical container was coupled with volume average thermal destruction kinetics of quality factor and center point destruction of a target microorganism (or F_a value). Modeling of such a process involves the mathematical description of (1) numerical solution of the two-dimensional heat conduction equation for a finite cylinder and (2) first order kinetics, describing the thermal destruction of microorganisms and quality change.

Heat Transfer Model. The heat flow in cylindrical geometry of finite shape was represented by the following partial differential equation (Ozisik 1989);

$$\partial^2 T / \partial r^2 + (1/r) \, \partial T / \partial r + \partial^2 T / \partial z^2 = (1/\alpha) \, \partial T / \partial t \tag{1}$$

where α is the thermal diffusivity and r and z are the radial and axial coordinates, respectively.

The initial and boundary conditions were;

$$\Gamma = \mathrm{Ti} \ \mathrm{at} \ \mathrm{t} = 0; \tag{2a}$$

$$\partial T/\partial r = 0$$
 at $r = 0$ and $t > 0$ (2b)

$$\partial T/\partial z = 0$$
 at $z = h/2$ and $t > 0$ (2c)

$$T = T_{\infty} \text{ at } r = a, z = 0, z = h \text{ and } t > 0$$
 (2d)

All thermophysical properties were assumed to be temperature independent, and the external heat transfer resistance at the can surface was considered to be negligible as in the case of processing of cans in steam. A finite difference computer program using Crank-Nicholson scheme for spatial derivatives and a fully implicit scheme for time derivative was employed (Ozisik 1989). Due to symmetry around both the axes of a cylindrical can, only one quarter of the cylinder was modelled using a 20×20 grid. Since an unconditionally stable implicit scheme was used, a time step size between 2 to 20 s was used depending on can size. The computer program was written in FORTRAN 77 to compute the transient temperature distribution in a cylindrical geometry.

Kinetics of Thermal Destruction. A primary objective of thermal processing is to achieve a preset level of commercial sterility. The intended process lethality (or thermal times), measured in terms of an F_o value, is used for this purpose:

$$F_{o} = \int_{0}^{t} 10 (T - T_{ref})/z_{m} dt$$
 (3)

where F_o is the integrated lethality (min); t is the time of processing (heating, holding and cooling), T is the temperature at the geometric center of can; T_{ref} is the reference temperature (121.1C) and z_m is the temperature sensitivity indicator of the thermal destruction of microorganism under consideration (typically, $z_m = 10C$ for spores of *Clostridium botulinum*). The integrated lethality was continuously computed and process simulation continued until the heating lethality reached the target value of 10 min. Based on the contribution

of lethality during the cooling, the computation process was then adjusted by trial and error to give a combined lethality (heating and cooling) of 10 min. Integrated heating time (F_{oq}) with respect to a quality attribute of food product was calculated at the reference temperature by:

$$F_{oq} = \int_{0}^{t} \frac{V}{[(1/V)} \int_{0}^{V} \frac{10}{10} (T - T_{ref})/z_{q} dv] dt$$
(4)

The above equation is similar to the F_o value except that the F_{oq} is based on volumetric/mass average destruction which is of greater interest for quality retention (e.g., nutrient retention). z_q indicates the temperature sensitivity indicator quality factor in question (used as a variable in this study). Using the calculated F_{oq} , the quality retention following a process can be obtained using the relationship:

$$\log N = \log N_o - [F_{oq}/D_{refq}]$$
(5)

where D_{refq} is the decimal reduction time for quality factor, N_o is initial quality and N is the quality remaining after processing. F_{oq} which determines the extent of retention of quality factors based on their respective D and z values, was used as a criterion for optimization in this study.

Variables Selection. Three factors, can size, thermal diffusivity, and z value of quality factor were used as variables in the study (Table 1). Other parameters (initial product temperature = 80C, retort come up time = 0 min, process lethality = 10 min and z value of microorganisms = 10C) were kept constant. A can has two-dimensions: radius (a) and height (h); in order to reduce the number of input variables for neural network analysis, a characteristic dimension was calculated using following equation (Ramaswamy *et al.* 1982):

Characteristic dimension =
$$(2.303)/[(2.467/(h/2)^2) + (5.783)/a^2]$$
 (6)

Thirteen operating temperatures were employed in the range 110 to 134C (at every 2C interval).

Calculation of Input/Output Data Needed. In order to construct and train the neural network, data on optimal process temperature, corresponding process time and associated quality factor were needed. These were obtained first by identifying the process times required at each of the 13 operating temperatures to achieve the preselected F_o value of 10 min. Simulation processes were run for these calculated times and the extent of quality factor destruction

THERMAL PROCESSING OPTIMIZATION				
Variables	No. of test levels	Range		
Can size	30	200 x 211 to 401 x 411 (30 can sizes) ¹		
Thermal diffusivity x 107 m ²	² /s 3	1.2 1.4 1.6		
z value of quality factors, C	4	15 25 35 45		
Temperature, C	13	110 to 134 C (2 C interval)		

TABLE 1. LEVELS AND RANGE OF INPUT VARIABLES USED IN THERMAL PROCESSING OPTIMIZATION

¹Lopez (1987)

for each z value was computed. From a plot of quality destruction vs. operating temperature, the optimal temperature for minimum quality destruction was obtained, again for each z value (representing arbitrary quality factor). The simulation was then rerun at this optimal process temperature to get exact process time and quality factor retention.

Neural Network. The software program employed was NEURALWORKS Explorer (NeuralWare Inc., Pittsburgh, PA). A four layer neural network (i.e., 1 input, 1 output and 2 hidden layers, the maximum that could be accommodated by the available software) was used in this study. The input layer consisted of 3 neurons which corresponded to 3 inputs variables (characteristic can dimension, thermal diffusivity of food product and z value of quality factor). The output layer also had 3 neurons one each for optimal sterilization temperature, process time and Foo. Standard back-propogation algorithm was used for learning/training of the network. In order to find the optimum configuration of neural network for the present problem, a range of 2 to 16 neurons in each hidden layer and 1,000 to 100,000 learning runs were tested. Then, the neural network was trained with 360 cases and its prediction capability was tested with same 360 cases. The optimum configuration was decided based on minimizing the difference between the neural network and the desired outputs. Once the optimum configuration with respect to number of neurons and learning runs was found, the performance of neural network was tested on different sizes of data set. The data set of 360 cases generated from finite difference simulation were randomly divided in two groups. The first group consisted of all 360 cases for learning and a randomly chosen 100 cases for the test. In second group, 100 cases were selected for learning and 100 cases for the test, all chosen randomly from the set of 360 cases. Several statistical parameters (mean absolute error,

standard deviation of error, mean relative error, standard deviation of relative error) were used for the determination of optimum number of neurons in hidden layer and also the number of learning runs. The following criteria were used with respect to the statistical parameters:

Error (ϵ) = | Finite difference output – Neural network response | Relative Error $(\epsilon_r) = (\epsilon/\text{finite difference output}) \times 100\%$ Mean Absolute Error (MAE) = Mean of ϵ values Standard Deviation of Error (SDE) = Standard deviation in ϵ values Mean Relative Error (MRE) = Mean of relative error (ϵ_r) Standard Deviation of Relative Error (SRE) = Standard deviation of relative error (ϵ_r)

The above parameters were used to give a broader range of selection criteria. The error magnitudes in user units (MAE, SDE in degrees C or min) are more meaningful with respect to process temperature and process times while the relative error (MRE, SRE in %) better describe the network performance with respect to F_{oq} .

RESULTS AND DISCUSSION

Computer Simulation

A total number of 4680 (13 temperatures ranging from 110 to 134C with interval of 2C for 360 test conditions) time-temperature simulations and associated quality changes were obtained to generate optimal processing parameters for 360 test conditions. The optimal sterilization temperature clearly dependent on the can size, thermal diffusivity and z value of the quality factor. Lower values of characteristic dimension of the can and higher values of thermal diffusivity resulted in higher optimal process temperature, probably due to resulting lower thermal gradients. This was also shown by Silva et al. (1992) while minimizing surface cook value. At higher z values (30 and 45C), the optimal sterilization temperatures were at the higher end of the range, while the opposite was true when the associated z values for quality factor were lower (15 and 25C). This was expected, since higher value of z_0 represents a more thermal resistant quality factor. Process time and F_{oq} were also significantly influenced (p < 0.05) by all three parameters. Process times were larger for the bigger can size and/or lower thermal diffusivity while quality retention was found to be higher (since lower F_{∞}) for smaller can size and/or higher thermal diffusivity. Process times were shorter with increasing z values since the associated optimal

process temperatures were higher. Average quality retention values have been reported to vary with z_q and a lumped parameter, f_h , which depends on can size and thermal diffusivity (Silva *et al.* 1992). In our study, we found that for smaller cans and lower thermal diffusivity, the optimal process temperatures were higher and nutrient retention values were lower at higher z_q values. However at higher thermal diffusivity, the nutrient retention data showed a curvi-linear trend, initially decreasing and then increasing with increasing z_q . With larger cans, on the other hand, irrespective of the thermal diffusivity value in the range studied, optimal process temperatures increased and the quality retention values decreased with z_q .

Learning/Training of Neural Network

Theoretically, once the neural network is learned/trained using the learning/training data, its performance can be evaluated by using the same data chosen in a random fashion (Huang and Mujumdar 1993). However, before the learning process, the optimum configuration of neural network should be determined since it has two variables: number of neurons in each hidden layer and number of learning runs. Several error parameters were used to determine adequacy of the neural network output response for a given input data set.

First, by keeping the number of learning runs constant (arbitrarily chosen as 50,000), the number of neurons in each hidden layer was varied from 2 to 16. The errors associated with optimal sterilization temperature as a function of the number of neurons are shown in Fig. 3. The calculated errors converged to a minimum value at 8 neurons in each hidden layer. Increasing the neurons beyond this level only resulted in increased computation time with no additional benefits. The trend was similar with the other two output responses, process time and F_{oq} , as well as other selected levels of learning runs demonstrating a minimum at 8 neurons. Magnitude of the deviations were, however, slightly higher for process time and F_{oq} .

In the next step, with the number of neurons in each hidden layer fixed at 8, the learning runs were varied from 1,000 to 100,000. The variations in different errors are compared in Fig. 4 as a function of learning runs, this time with process time shown as an example output.

The convergence was observed at about 50,000 learning runs beyond which the changes were small. The trend with respect to errors was again similar for the other two output responses, optimal sterilization temperature and F_{oq} with some differences in their magnitudes.

Neural network configuration with 8 neurons in each hidden layer and 50,000 learning runs was evaluated for performance testing on the two sets of data (first set: all 360 cases for learning and 100 cases for testing; second set:



FIG. 3. ERROR PARAMETERS AS A FUNCTION OF NUMBER OF NEURONS FOR OPTIMAL STERILIZATION TEMPERATURE (360 CASES FOR LEARNING AND 360 CASES FOR TESTING) WITH 50,000 LEARNING RUNS

100 randomly selected cases for learning and another 100 randomly selected cases for testing). The error parameters were compared with the reference set where all 360 cases were used for both learning and testing.

The prediction performance of the neural network for the two sets is shown in Fig. 5-7 as plots of neural network predicted values vs. desired output values for all three variables. The predicted values were more evenly and tightly distributed around the regression line for the first set involving higher number of learning cases (360). For the second set involving lower number of learning cases (100) the predicted values generally showed more scatter with deviation at both ends.

The associated errors with the neural network outputs are compared in Table 2. The observed high R^2 values (>0.98) indicated excellent correlations of neural network predicted values with the finite difference output. Relatively, slightly lower correlations were observed while predicting the changes in quality factors (F_{oq}). The magnitude of errors for the first set was nearly the same as those for the reference set for all three outputs. However, with the second set,



FIG. 4. ERROR PARAMETERS AS A FUNCTION OF LEARNING RUNS FOR PROCESS TIME (360 CASES FOR LEARNING AND 360 CASES FOR TESTING) WITH 8 NEURONS IN EACH HIDDEN LAYER

the errors were of similar magnitude compared to the errors of reference set for the optimal sterilization temperature and process time, while for F_{oq} , they were relatively higher, especially with reference to relative error (MRE) and standard deviation of relative error (SRE). The deviation in optimal process temperature prediction (MAE) was essentially of same magnitude (0.35±0.32C) for both training sets. The mean relative error in process times was about 5.2% with both training sets; however, the standard deviation of relative error was ~5% with first training set and ~7% in the second training set. The relatively large standard deviations associated with process time predictions by neural network were due to deviations observed under conditions of low (<30 min) and high (>100 min) process times. The mean relative error with F_{oq} was ~2.5% for the first set and ~4.5% for the second set. Neural network prediction showed



FIG. 5. CORRELATION OF NETWORK OUTPUT FOR OPTIMAL STERILIZATION TEMPERATURE USING DIFFERENT SIZE OF LEARNING CASES

deviation from the desired output mostly at the higher end of F_{oq} values for the first set where 360 cases were used for learning purpose. However, when only 100 cases used for learning, the predicted values deviated at both ends (Fig. 7). These results demonstrate that the accuracy of neural network predictions increases as the availability of input data increases.

Overall, the relative errors associated with the process time prediction were the highest and those associated with the process temperature were the least



FIG. 6. CORRELATION OF NETWORK OUTPUT FOR PROCESS TIME USING DIFFERENT SIZE OF LEARNING CASES

somewhat in proportion to the range of values (optimal process temperature from 112 to 132C, process time from 20 to 165 min and F_{oq} from 20 to 90 min) employed for these variables. On a percentage basis compared to the midpoint values, the range associated with process times was $\pm 80\%$, while the same with process temperature was only $\pm 9\%$. With F_{oq} , the range was $\pm 60\%$. These differences are also due to the logarithmic nature of both process time and



FIG. 7. CORRELATION OF NETWORK OUTPUT FOR F_{oq} USING DIFFERENT SIZE OF LEARNING CASES

quality factor retention in relation to optimal process temperature. In neural network weights were adjusted to result simultaneously in minimum error in prediction of all three parameters, which are different in their nature. The relative errors found were on an average within 5% of the above ranges. In general, these errors will have an even smaller influence on quality factor retention in real processing conditions. For example, the neural network prediction error of $\pm 5\%$ at lower end of F_{oq} values would mean $\pm 1.2\%$ error

Statistical Parameters	Reference group ¹		,1 F	First Group ²			Second Group ³		
	*opt		• oq	- opt		• 0q	• opt		• oq
R ²	0.993	0.988	0.992	0.994	0.986	0.989	0.992	0.985	0.981
MAE	0.368	3.122	0.806	0.328	3.305	1.039	0.383	3.187	1.700
SDE	0.345	2.859	0.949	0.307	2.893	1.521	0.335	2.957	1.455
MRE	0.303	4.827	2.108	0.269	5.168	2.490	0.315	5.254	4.583
SRE	0.280	4.838	2.206	0.252	4.996	2.632	0.272	6.802	4,528

TABLE 2. COMPARISONS OF ERROR PARAMETERS FOR DIFFERENT SIZE OF LEARNING AND TEST CASES

¹learning = 360 cases and test = 360 cases

 $\frac{2}{2}$ learning = 360 cases and test = 100 cases

³learning = 100 cases and test = 100 cases

in thiamine retention [$F_{oq} = 23.6$ min, $D_{ref} = 163$ min (Lund 1975), z = 25C, can size = 202 × 204, thermal diffusivity = 2.0 × 10⁻⁷] at 123C and at higher end of F_{oq} values $\pm 1.9\%$ error [$F_{oq} = 69.6$ min, $D_{ref} = 163$ min, z = 25C, can size = 401 × 411, thermal diffusivity = 1.2×10^{-7}] at 115C.

CONCLUSION

The prediction of optimal sterilization temperatures, and their corresponding process time and F_{oq} values using an artificial neural network is presented. The neural network predicted all three outputs simultaneously, unlike conventional regression models where three different equations are needed. The study showed that the number of neurons in each hidden layer and the learning runs need to be optimized before using the neural network. For the present problem, a neural network with 8 neurons in hidden layers and 50,000 learning runs was found optimum for its performance. The trained network was found to predict responses with less than 5% associated errors with respect to optimal sterilization temperature, process times and quality factor retention.

NOMENCLATURE

a	Radius of a can, m
d	Desired resonse of neuron
D	Decimal reduction time, min
f _h	Heating rate index, min
F,	Process lethality, min
h	Height of a can, m
Μ	Layer number
MAE	Mean absolute error
MRE	Mean relative error
N	Quality factor
PT	Process time, min
r	Radial coordinates
S	Output of neuron
SDE	Standard deviation of error
SRE	Standard deviation of relative error
t	Time, s
Т	Temperature, C
V	Volume, m ³
w	Weight coefficient
W	Set of weight coefficients
х	Input
Х	Set of inputs
Z	Axial coordinates, Temperature sensitivity indicator, C

Greek Symbols

α	Thermal	diffusivity
E	Error	

Subscripts

0, 1	Integer numbers
i, o	Initial
m	Microorganism
opt	Optimal
q	Quality
ref	Reference
œ	Heating medium

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