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Using artificial neural networks to predict thermal conductivity of pear juice

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Abstract

Thermal conductivity is an important property of juices in the prediction of heat- and mass-transfer coefficients and in the design of heat- and mass-transfer equipment for the fruit juice industry. An artificial neural network (ANN) was developed to predict thermal conductivity of pear juice. Temperature and concentration were input variables. Thermal conductivity of juices was outputs. The optimal ANN model consisted 2 hidden layers with 5 neurons in first hidden layer and the second one has only one neuron. The ANN model was able to predict thermal conductivity values which closely matched the experimental values by providing lowest mean square error (R^2=0.999) compared to conventional and multivariable regression models. However this method also improves the problem of determining the hidden structure of the neural network layer by trial and error. It can be incorporated in heat transfer calculations during juices processing where temperature and concentration dependent thermal conductivity values are required.

Keywords: Artificial Neural Network, Thermal conductivity, Fruit juices, Pear

Introduction

Thermal conductivity is an important property of juices in the prediction of heat- and mass-transfer coefficients and in the design of heat- and mass-transfer equipment for the fruit juice industry. Accurate thermal conductivity data and their variation with operating conditions (over wide temperature and concentration regions) are needed for various research and engineering applications in any branch of the food industry, such as developing food processes and processing equipment, the control of products, filters, and mixers, engineering calculations on evaporation rates, pumping, and pipe requirements, mixing requirements, quality evaluation; and an understanding of the structure of food and raw agricultural materials (Magerramov *et al*. 2006).

As the thermal conductivity of juices strongly depend on concentration and temperature, and due to natural differences between the fruits, it is nearly impossible to experimentally determine and tabulate the thermal conductivity of fruit juices for all possible conditions and compositions. However, most existing thermal conductivity measurements for fruit juices are at room temperature and very limited concentration range. Therefore an appropriate correlation and prediction models for the thermal conductivity of juices, as a function of temperature and concentration, to cover the entire range of temperature and concentration is necessary.

For this reason there has been consistent effort spent in developing generalized correlations to predict thermal properties of food materials for the use in process design and optimization. In recent years, mathematical modeling and computer-based numerical analyses have become the main tools for understanding and predicting processing phenomena.

Magerramov *et al*. (2006) have been presented and modeled thermal conductivity data as a function of concentration and/or process temperature. They also proposed 5 semi theoretical methods for the prediction of thermal conductivity of pear juice. Among them, the multi parametric Model (equation 1) with AAD = 0.1 to 0.2 %, where AAD is the average absolute deviation)) is best represented by the present experimental

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thermal conductivity data, but the predicting capability of equation 2 (AAD = 0.6 to 0.7%) is much better than that of others. Moreover, in this equation the minimum experimental thermal conductivity information at a reference temperature is needed to predict the values of the thermal conductivity of juices at high temperatures. Equation 2 can be recommended to calculate the combined effects of the temperature and concentration on the thermal conductivity of juices over wide ranges of temperature and concentration just using the values of thermal conductivity at reference temperature T0. It was found that the prediction equation 1 and 2 can be adopted with satisfaction.

$$\lambda(T,x) = 0.5794 - 3.7520 \times 10^{-3}x + (9.6237 \times 10^{-4} - 7.5953 \times 10^{-7}x)T + (-2.7390 \times 10^{-6} + 2.2198 \times 10^{-8})T^2 \quad (1)$$

$$\frac{\lambda(T,x)}{\lambda(T_0,x)} = \left(\frac{T}{T_0}\right)^m \quad (2)$$

Where λ is the thermal conductivity, x is the concentration, and T is the temperature, could be adopted with satisfaction.

Artificial Neural Network (ANN) modeling is increasingly accepted and is an interesting method for the estimation and prediction of food properties and process related parameters. Several researchers used Artificial Neural Network technique for predicting thermal conductivity of fruits and vegetables, bakery products and foods (Hussain and Rahman, 1999; Mittal and Zhang, 2000; Sablani *et al*., 2002; Sablani and Shafiur Rahman, 2003; Hussain and Shafiur Rahman, 2003; Rai *et al*., 2005a,b; Shafiur Rahman *et a*l., 2012).

However, little work has been conducted on the prediction of thermal conductivity of fruit juices using ANN. Consequently, the objective of this work was to develop an ANN model to predict the thermal conductivity of pear juice of known temperature and composition. Comparisons of the thermal conductivity prediction by ANN with the conventional analytical model described in the literature have also been made in this work.

Materials and methods

Experimental methods

Experimental data

Many researchers have measured thermal properties of fruit and vegetable juices such as thermal conductivity byvarious techniques. Thermal conductivity data needed for development of the ANN model were obtained from the thermal conductivity data set of pear juice (66 samples) were prepared by Magerramov *et al.* (2006). A total of 66 data points for pear juice at a temperature range of 20 to 120 °C and concentrations up to 50 °Brix were used (Table 1). According to Table 1, the thermal conductivity of pear juice considerably increases with temperature.

Model development

The development of a neural network model involves: the generation of (or compilation of available) data required for training/testing, the training/testing of the ANN model, the evaluation of the ANN configuration leading to the selection of an optimal configuration, and validation of the optimal ANN model with a data set not used in training before. The flow chart of methodology for developing ANN architecture is described in Figure 1.

Artificial Neural Networks (ANN)

Artificial Neural Networks (ANN) provides a range of powerful new techniques for solving problems in sensor data analysis, fault detection, process identification and control. The major advantages of using an ANN model are that it works only with input - output data, does need a well-defined algorithm to convert an input into an output, but a representative collection of examples is necessary to offer the desired output(Heaton, 2005).A single model can be used to generate multiple outputs. Once the neural network model has been adequately trained and validated, it is able to make predictions on new set of input data, but not used in the developing of the model (Curteanu, 2011). Due to their capabilities, ANNs can be used on a wide range of processes and systems from various domains (Kamali, M. Mousavi,

2008, Pirdashti *et al*.2013).Basic component of a neural network is the neuron, also called "node". Figure 2 illustrates a single node of a neural network. The inputs are represented by a1, a2 and an, and the output by Oj. There can be many input signals to a node. The node manipulates these inputs to give a single output signal (Lübbert and Simutis, 1994).

The values w_{1j} , w_{2j} , and w_{nj}, are weight factors associated with the inputs to the node. Weights are adaptive coefficients within the network that determine the intensity of the input signal. Every input (a_1, a_2, . . .,a_n) is multiplied by its corresponding weight factor (w_{1j}, w_{2j}, . . . , wnj), and the node uses summation of these weighted inputs (w_{1ja1}, w_{2ja2}, . . . , wnjan) to perform further calculations. In the initial setup of a neural network, weight factors usually are chosen randomly according to a specified statistical distribution. The other input to the node, bj, is the node's internal threshold, also called bias. This is a randomly chosen value that governs the node's net input through the following equation (Nasr *et al*., 2012):

$$u_i = \sum_{i=1}^{n} (w_{ij} * a_i) + b_j \qquad (3)$$

The node's output is determined using a mathematical operation on the node's net input. This operation is called a transfer function. The transfer function can transform the node's net input in a linear or non-linear manner. In the present work Sigmoid transfer function was applied:

$$f(x) = \frac{1}{1 + e^{-x}} \qquad 0 \leq f(x) \leq 1 \qquad (4)$$

The neuron's output, O_j, is found by performing one of this function on the neuron's net input, u_j. Neural networks are made of several neurons that perform in parallel. The weight factors and thresholds are adjusted in training process. Training is the process by which the weights are adjusted systematically so that the network can predict the correct outputs for a given set of inputs (Sadrzadeh et al. 2009). There are many different types of training algorithms. From all the types of networks enumerated above, feed-forward multilayered networks (multilayer perceptron, MLP) is the most used because is general and simply to apply (Wilamowski, 2009). In addition, advantages of MLP are also the easiness of programming and good results often provided (Fernandes and Lona, 2005). In the mathematical field, the universal approximation theory (Cybenko theorem) states that the standard MLP with a single hidden layer that contains finite number of neurons with arbitrary activation functions are universal approximate on a compact subset of R^n, property which makes it attractive to various researchers. MLP is composed of an input layer with a number of neurons corresponding to the input variables, one or more hidden layers and an output layer whose number of neurons corresponds to the number of output variables. Figure 3 shows the structure of this kind of ANN.

Table1- Experimental thermal conductivities (Wm-1K-1) of pear juices as a function of temperature for various concentrations Magerramov et al. (2006).

	Concentration(°Brix)					
T(K)	14	19	25	30	40	50
293.15	0.545	0.526	0.503	0.485	0.450	0.408
303.15	0.553	0.535	0.511	0.493	0.458	0.417
313.15	0.561	0.543	0.519	0.500	0.466	0.425
323.15	0.568	0.551	0.526	0.508	0.473	0.433
333.15	0.575	0.558	0.534	0.514	0.480	0.441
343.15	0.581	0.565	0.540	0.521	0.487	0.448
353.15	0.587	0.571	0.547	0.527	0.493	0.456
363.15	0.593	0.576	0.553	0.532	0.499	0.462
373.15	0.598	0.581	0.559	0.538	0.504	0.469
383.15	0.603	0.585	0.564	0.542	0.508	0.476
393.15	0.607	0.589	0.568	0.547	0.513	0.481

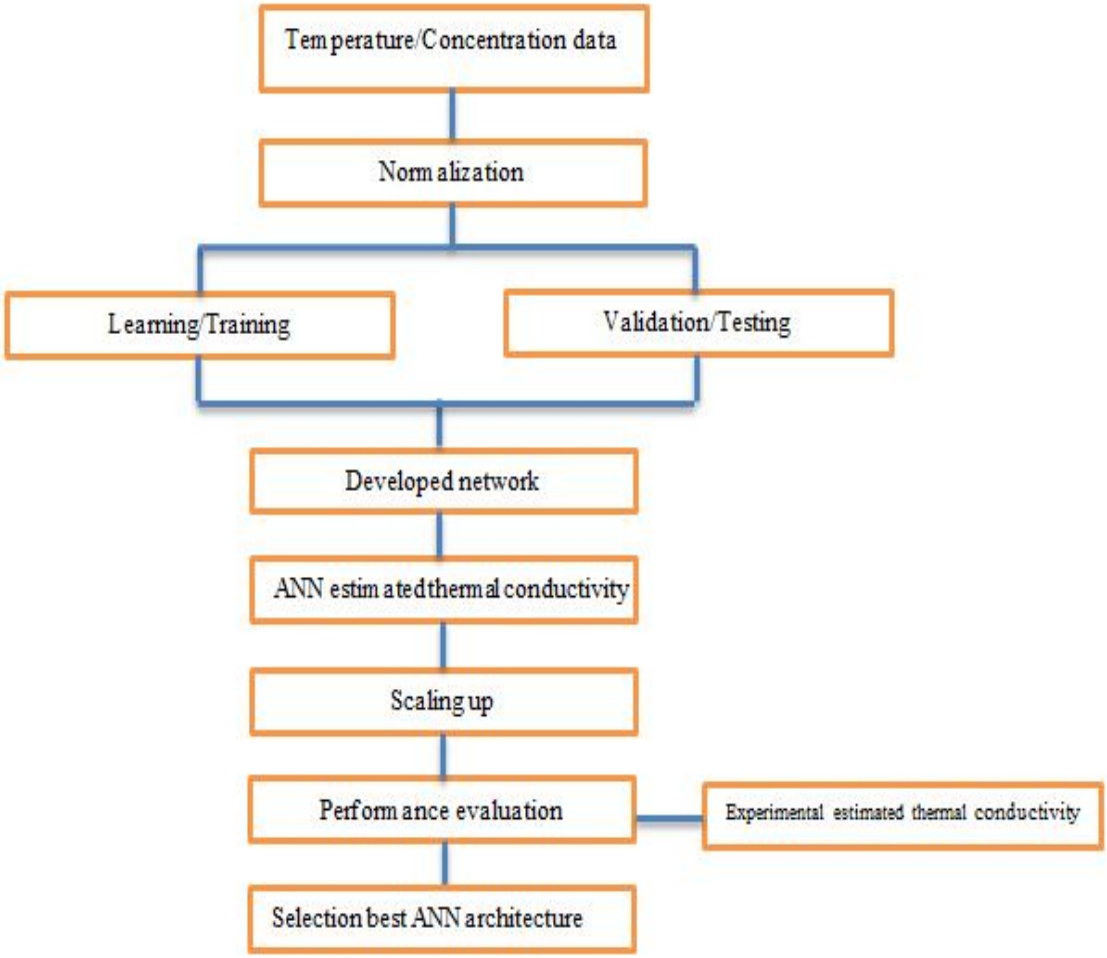

Figure1. Methodology for developing ANN architecture

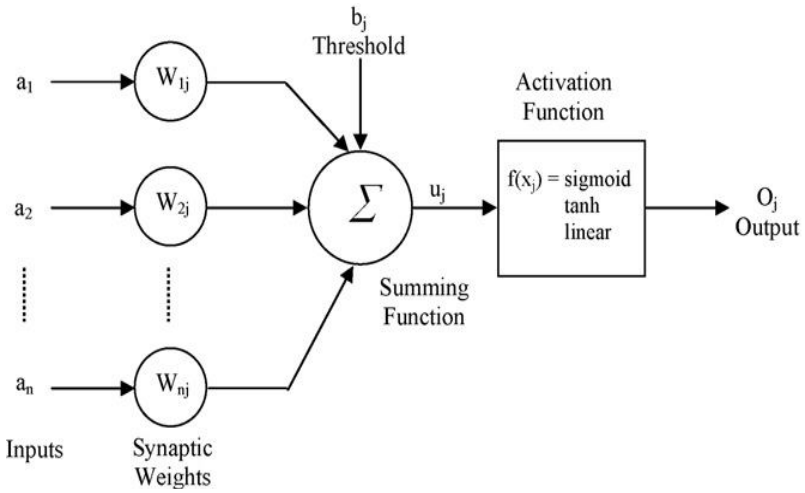

Figure2. Single node anatomy (Sadrzadeh *et al.*, 2009).

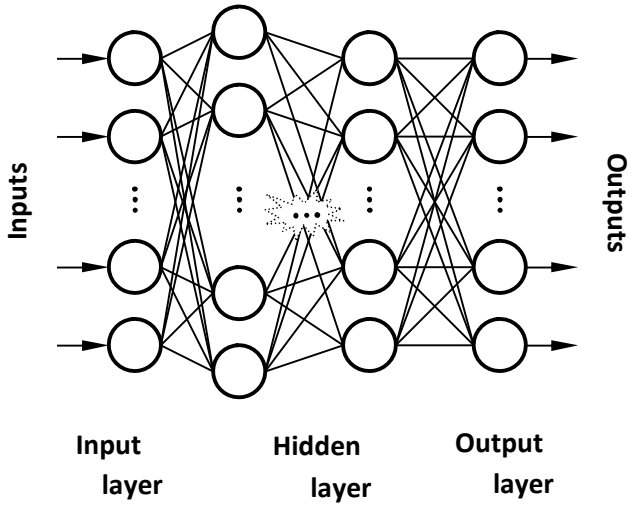

Figure 3. Structure of multilayer perceptron

Concerning the number of layers and neurons, several considerations have to be taken into account. Using a single hidden layer, a given degree of accuracy is attained only in the limited cases as the number of nodes becomes very large. For most complex cases, additional layers are necessary for a good fit and an improved generalization capability (Fernandes and Lona, 2005, Pirdashti *et al.* 2013). One of the most common classes of training algorithms for feed-forward neural networks is called back propagation (BP). Many other methods have been developed based on BP. Three subsets of data are used to build a model: training, validation and testing subsets. Training data set is used in training procedure. Validation data set is used to check the generality of network. If the network is trained sufficiently, the network output will differ only slightly from the actual output data. In initial steps of training, errors of both training and validation data are reduced. After several steps, the error of training data decreases while that of validation data increases. As a result, the network is over trained and its generality decreases. Hence, the training process must be continued until the validation data error decreases. Testing data set is used to test the trained network for unseen patterns (whose results are known for researcher but not used in training procedure). The network generalizes well when it sensibly interpolates these new patterns (Sadrzadeh *et al.* 2009).

For the prediction of thermal conductivity of pear juice, a feed-forward multi-layer neural network with input, output and hidden layers was used in this study which is shown in Figure4.

Results and Discussion

Based on ANN model, the input layer has 2 neurons and the output layer has only one neuron. Hidden layers are composed of two layers that the second one has only one neuron. The number of the neurons in the first hidden layer has to be selected by trial and error to minimize the mean relative error between the actual and the predicted thermal conductivity. In this study, the Levenberg-Marquardt algorithm with five neurons in the hidden layer was used to train the network. The network uses the sigmoid transfer function in the hidden layer, the linear activation function in the output layer.

Seventy present of data (46 samples) were randomly selected to train the network and 15 % (10 samples) were used for validation process and the remaining 15% were used for testing process. In the study, two hidden layer nodes were chosen to select the best production results. To reveal the credibility of prediction from the optimal ANN, predicted versus experimental values of thermal

conductivity was plotted (Figure 5). The results demonstrate very good agreement between the predicted and the experimental values of thermal conductivity ($R^2 = 0.999$).

Also, some statistical parameters are used for better comparison of the models. These statistical parameters are Normalized Bias (NB), Standard Square Error (SSE), Mean Square Error (MSE), Root Mean Square Error (RMSE) and *R*-square (R^2) which are described in Equations (6)–(10) (Draper and Smith (1998)., Armstrong and Collopy (1992)., *Cameron et al., 1997)*. They are used for the fitness investigation and error determination of the ANN model compared to equation 2.

where n is the number of experimental points; y_i^{exp} and y_i are the experimental and predicted values of thermal conductivity,respectively.Quantitative comparisons of the models using these statistical parameters are summarized in table 2, respectively.

$$NB = \sum_{i}^{n} \frac{(y_i - y_i^{exp})}{y_i^{exp}} \times 100 \quad (6)$$

$$SSE = \sum_{i}^{n} (y_i - y_i^{exp})^2 \quad (7)$$

$$MSE = \sum_{i}^{n} \frac{(y_i - y_i^{exp})^2}{n} \quad (8)$$

$$RMSE = \sqrt{\sum_{i}^{n} \frac{(y_i - y_i^{exp})^2}{n}} \quad (9)$$

$$R^2 = \frac{\sum_i^n (y_i^{exp} - y_{mean})^2 - \sum_i^n (y_i - y_i^{exp})^2}{\sum_i^n (y_i^{exp} - y_{mean})^2} \quad (10)$$

Table 2. Prediction accuracy of the models developed from the data set

	Statistical parameters				
	NB	SSE	MSE	RMSE	R^2
Model					
Eq.1	-9.6632	3.61×10^{-1}	5.4642×10^{-3}	7.392×10^{-2}	0.985
Eq.2	-0.1657	6.4625×10^{-4}	9.7916×10^{-6}	3.129×10^{-3}	0.996
ANN	-0.0037	1.454×10^{-5}	2.2028×10^{-7}	4.693×10^{-4}	0.999

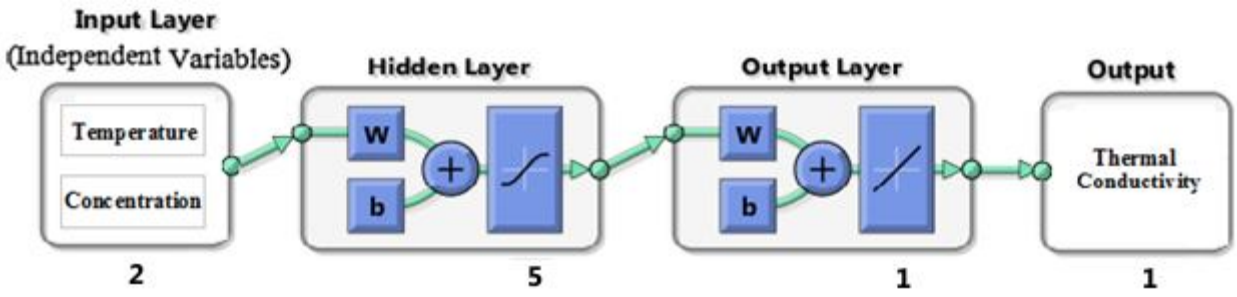

Figure 4. Schematic of multilayer neural network used to predict the thermal conductivity of pear juice

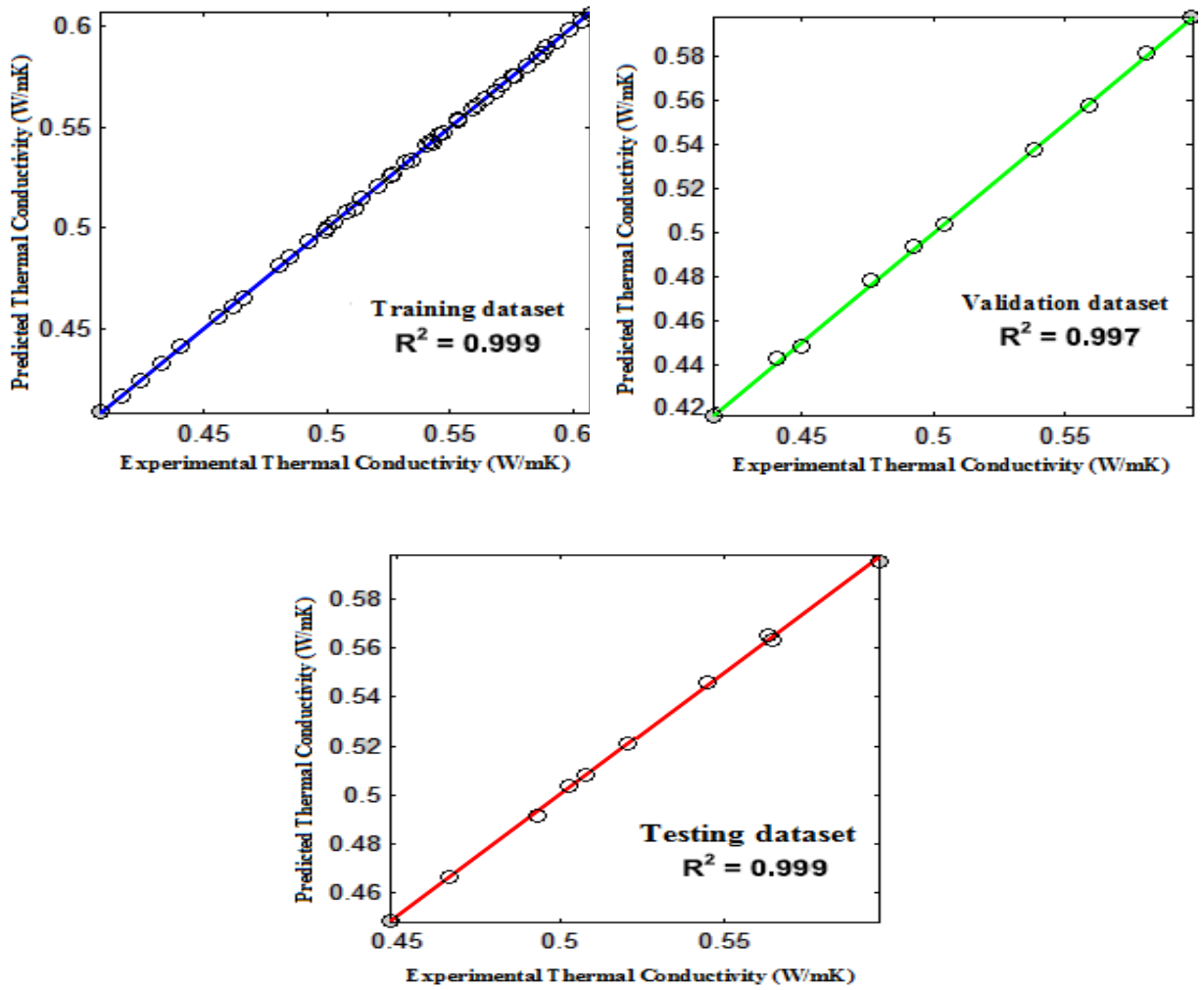

Figure 5. Correlation of experimental versus neural network values of thermal conductivity with training, validation and testing data set

Conclusion

A neural network based model was developed for the prediction of thermal conductivity of pear juice under a wide range of conditions of temperature and concentration. The optimal model, which consisted of 2 hidden layers and 5 neurons in first hidden layer, was able to predict thermal conductivity values. Empirical model was less accurate compared to neural network model in predicting the thermal conductivity. The ANN model can predict thermal conductivity of other juices when database be available.

where n is the number of experimental points; y_i^{exp} and y_i are the experimental and predicted values of thermal conductivity,respectively.Quantitative comparisons of the models using these statistical parameters are summarized in table 2, respectively.

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استفاده از شبکه های عصبی مصنوعی برای پیش‌بینی هدایت حرارتی آب گلابی

زینب رفتنی امیری*[۱]، هنگامه درزی اربابی[۲]

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چکیده

هدایت حرارتی، یکی از ویژگی های مهم آب میوه ها برای پیش بینی ضرایب انتقال جرم وحرارت و هم چنین طراحی تجهیزات انتقال جرم و حرارت در صنعت آب میوه می باشد. شبکه عصبی مصنوعی برای پیش بینی هدایت حرارتی آب گلابی توسعه داده شد. دما و غلظت متغیرهای ورودی و هدایت حرارتی آب میوه متغیر خروجی بودند. مدل بهینه این شبکه شامل دو لایه پنهان با ۵ نرون در لایه اول و یک نرون در لایه دوم بود. مدل شبکه مصنوعی توانست مقادیر هدایت حرارتی را بسیار نزدیک به مقادیر اندازه گیری شده در آزمایش پیش بینی کند و در مقایسه با مدل های متعارف و رگرسیون چند متغیره از پایین ترین مجذور خطای میانگین (R^2=0.999)برخوردار بود. به علاوه با بکارگیری این روش می توان ساختار پنهان لایه ها در شبکه های عصبی را از طریق آزمون و خطا تعیین کرد.این روش می تواند در محاسبات انتقال حرارت در فراوری انواع آب میوه، جایی که نیاز به محاسبه هدایت حرارتی بر حسب دما و غلظت باشد، به خوبی مورد استفاده قرار گیرد.

واژه‌های کلیدی: آب میوه، شبکه عصبی مصنوعی، گلابی، هدایت حرارتی

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