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Prediction of Trans-anethole Extraction Yield from *Pimpinella Anisum* Seeds Using Artificial Neural Network

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Abstract

In this investigation, the extraction of trans-anethole (t-anethole) using subcritical water solvent was employed as a case-study. A feed-forward multilayer back propagation artificial neural network (ANN) with various train algorithms and number of neurons was considered for the prediction of t-anethole extraction yield (mg/g dry sample). The input variables were temperature (100-175 °C), flow rate (0.5-4 ml/min), mean particle size (0.25-1 mm) and output was t-anethole extraction yield. The optimization of neural network structure is manufactured based on minimum mean square error (MSE) of training and testing data. The optimal ANN model is composed of one hidden layer with five neurons. The prediction of t-anethole extraction yield using the ANN model was confirmed to be an accurate, appropriate and simple method.

Keywords: Trans-anethole, Extraction, Subcritical Water, ANN model.

INTRODUCTION

T-anethole is a predominant part of *Pimpinella anisum* seeds and it is commonly available as a proper source [1]. It is important to choose the suitable extraction technique for feasible maximum extraction yield because valuable compounds in plant seeds usually are in low concentrations. The traditional extraction techniques such as solvent extraction and hydrodistillation have a few tunnable factors to control the extraction processes selectivity. Therefore usage of alternative extraction techniques with better selectivity and efficiency is highly appropriate [2].

Subcritical water, known also as hot water pressurized, is the preferred choose in comparison with traditional solvents when the extract has preferable species. This method commonly has a high selectivity power of valuable compounds [3-6]. Recently the applications of subcritical water extraction (SWE) for various matters such as essential oils and bioactive component have been developed [7-9]. There are many experimental works with SWE but threre are not significant researches on modeling of extraction process.

The current models for process are based on the thermodynamic distribution coefficient (K_D), analogous to the hot ball heat transfer mode and differential mass balances along the extraction bed [10].

Nowadays, artificial neural networks (ANNs) bave been used as computationally efficient methods. The ANNs are widely used for prediction of food properties and process-related parameters [11-15]. Also, it has been successfully applied for modeling and optimization of different problems of chemical engineering. One of the great advantages of this method is that no mathematical model is required.

The purpose of this study is to model the t-anethole extraction yield using subcritical water by ANN based on the experimental data in a previous work [16]. In this aspect, there is no ANN model available to predict the yield of SWE.

Artificial Neural Network

A network typically contains connected nodes, which represent the neuron body. The nodes are connected by links that perform like axons and dendrites of their biological counterpoints [17]. An ANN influenced by the human brain functioning systems is a forceful data modeling tool. It is a specifically effective algorithm that learns the relationships between the input and the output vectors to approximate any function with irregularities. The more nonlinear and complicated systems were successfully modeled by this technique [18,19]. The ANN is the multilayer neural network where the neurons are set into three layers: input layer, hidden layer, and output layer.

The multi-layer perceptron (MLP) network construction is one of the most usually applied ANN and it was appropriate for modeling of the supercritical extraction of essential oils [20]. Fig. 1 describes the MLP network, which contains an input layer with 3 neurons, an output layer with one neuron, and one hidden layer with 5 neurons.

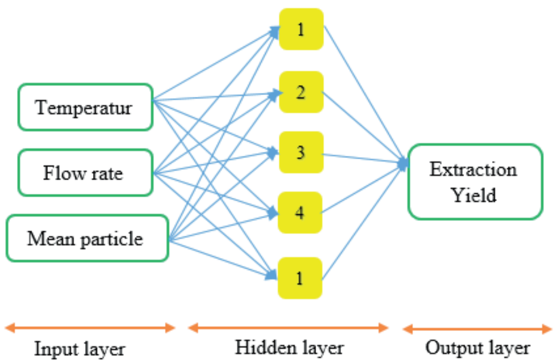

Fig. 1. A diagram of ANN formation for SWE of t-anethole.

The normalized input data are transferred into the input layer and then transmitted from the input layer to the hidden layer and eventually attain the output layer of the network [21]. Initially, every node in the hidden or output layer performances as a summing junction which incorporates and rectifies the inputs from the prior layer as follows:

$$Y_i = \sum_{k=1}^{i} P_i W_{ik} + b_k \quad (1)$$

Wherever Y_i is the net input to node k in hidden or output layer, P_i is the inputs to node k (or the outputs of the prior layer), W_{ik} is the weights representing the strength of the connection between the i^{th} node and k^{th} node, i is the number of nodes and b_k is the bias related to node k. every neuron contains a transfer function representing an internal activation level. The output from a neuron is specified by changing its input using a appropriate transfer function [21,22]. The transfer functions for function estimation usually are linear function, hyperbolic tangent and sigmoidal function [23]. The past studies confirmed that the sigmoidal function is the most famous transfer function for a non-linear relationship [24]. The common formula of this function is specified below [25]:

$$O_k = \frac{1}{1 + \exp(-Y_i)} \quad (2)$$

Where the output of node k is O_k. That is an component of the inputs to the nodes in the next layer. There are different back propagation algorithms inclusive the levenberg-marquardt (LM), scaled conjugate gradient (SCG) and gradient descent with variable learning rate back propagation (GDX). The suitable algorithm was selected with trial and error.

Ann Model Description

To predict extraction yield for subcritical water extraction of t-anethole a feed-forward multi-layer neural network was employed. The temperature (P_1), flow rate (P_2) and mean particle size (P_3) were used as inputs, and the t-anethole extraction yield was used as output. The experimental data were according to a Box-Burman design [16], by iterative training of the different ANN constructions using the following general approach. The experimental results were at random separated into two groups. One group was assumed as training data and another group was applied as testing data in this model. For a investigative decision of the best ANN construction of lowest error these experimental data were used as training data. The number of nodes was changed from 3 to 8 in the hidden layer to discovery an ANN construction that explain the extraction yield with the lowest error.

As illustrated in Fig. 1, ANN was used to develop a prediction model to predict the t-anethole extraction yield of SWE. The Inputs and output are normalized (range of 0–1) for the decline of network error and higher homogeneous results as follows:

$$P_{norm} = \frac{p - p_{min}}{p_{max} - p_{min}} \quad (3)$$

Where p_{min}, p_{max}, p, P are minimum, maximum, actual and normalized values respectively. The values of the interconnection weights are specified by the training method with a group of data. The object is to discover the value of the weight that minimizes the error. The manner of the employed network was checked with the mean squared error (MSE) and the coefficient of determination (R^2) as follows:

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (Y_i - Y_{ai})^2 \quad (4)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (Y_i - Y_{ai})^2}{\sum_{i=1}^{n} (Y_{ai} - Y_m)^2} \quad (5)$$

The number of runs is n, the predicted value obtained from the ANN model is Y_i, the actual value is Y_{ai} and the average of the actual values is Y_m.

RESULTS AND DISCUSSION

The experimental data of t-anethole extraction yield via subcritical water at 100-175 °C, 0.5-3 ml/min and 0.25-1 mm have been given in an accepted paper [16]. Three input variables were temperature (p_1), flow rate (p_2) and mean particle size (p_3) at three levels 0, 0.5 and 1. By varying the number of neurons in the hidden layer and network training algorithm the network implementation was optimized to attain the finest match of the training data with the experimental data. The experimental data of the three parameters and three levels used for BBD, the results for t-anethole yield extracted and predicted values by ANN model are shown in Table 1.

The relative error has been employed for evaluating the results and model predictions as well. The percentage of relative error is explained as:

$$\text{Relative Error (\%)} = \frac{\text{Exp. data} - \text{Pre. data}}{\text{Exp. data}} \times 100 \quad (6)$$

The experimental data employed to create the model is "Exp. data" and the output of the neural networks at the same conditions is "Pre. data". The convergence of relative error to zero is the better result. In Table 1 (derived from ANN model for training and testing data, respectively) the error of measurements with this standard has been displayed in Table 1. The It is evident that the neural network model has a better overlap with the Exp. data. The three-layer neural network model used to predict t-anethole extraction yield has three inputs, 3-8 hidden neurons, and one output.

Table 1. Design of experiment and results of t-anethole yields extracted by subcritical water (p: independent variable and P: normalized variable.)

Run	Temperature T (°C) p_1	P_1	Flow rate Q (ml/min) p_2	P_2	particle size d_p (mm) p_3	P_3	Amount of t-anethole (mg/g) [19]	Predicted value by ANN (mg/g)	Relative error
1	175	1	1.75	0.5	0.25	0	2.0141	2.0230	0.0044
2	138	0.5	3	1	0.25	0	2.4979	2.3325	0.0946
3	175	1	3	1	0.6	0.5	2.4461	2.6869	0.0984
4	138	0.5	1.75	0.5	0.6	0.5	1.5792	1.5792	0.00001
5	138	0.5	1.75	0.5	0.6	0.5	1.5792	1.5792	0.00001
6	138	0.5	0.5	0	1	1	0.135	0.1350	0.00001
7	100	0	1.75	0.5	0.25	0	0.6121	0.6076	0.6732
8	138	0.5	1.75	0.5	0.6	0.5	1.5792	1.5792	0.00001
9	100	0	3	1	0.6	0.5	0.9096	0.9096	0.00001
10	100	0	1.75	0.5	1	1	0.5082	0.5082	0.00001
11	100	0	0.5	0	0.6	0.5	0.3003	0.3003	0.00001
12	138	0.5	3	1	1	1	1.9961	1.9961	0.00001
13	138	0.5	0.5	0	0.25	0	0.5978	0.2343	0.6080
14	175	1	0.5	0	0.6	0.5	0.7369	0.7369	0.00001
15	175	1	1.75	0.5	1	1	1.0410	1.0410	0.00001

It is known that the number of neuron in hidden layer is very important. If very few neurons are in hidden layer, the efficiency of the network will not be acceptable. On the other hand, if too many neurons be in the hidden layer, the training will be very long and may be over-fitting [23-25]. The standard employed to choice the suitable ANN model contained choosing the number of neurons, which gave a minimum final mean square error during the training and testing of the ANN. In this study, the best prediction performance of the ANN model was chosen by six structures (one hidden layer with three to eight neurons). The network uses the sigmoid transfer function in the hidden layer, the linear activation function in the output layer, and different training algorithms (LM, SCG and GDX) as a training algorithm. ANN has been trained with 75% of the dataset and 25% of the data have been applied for testing the predictions of it.

Table 2 describes errors and correlation coefficients of train and test in the model versus the number of neurons on the hidden layer for different training algorithms. It was cleared that the structure of one hidden layer with four neurons and LM train algorithm resulted in the minimum error. Therefore, the optimal ANN model configuration was the network of one hidden layer with five neurons. The optimum number of hidden layer neurons was determined to be five for this network. Two scatter plots of experimental data against the predicted values by ANN model were shown in Figs. 2 and 3.

Table 2. Optimization of number of neurons for various neurons and algorithms.

	Neuron no.	MSE[b]		
Train algorithm [a]		LM	SCG	GDX
Training	3	4.41×10^{-16}	6.59×10^{-13}	9.83×10^{-13}
	4	1.69×10^{-15}	9.62×10^{-13}	9.96×10^{-13}
	5	1.7×10^{-18}	5.62×10^{-13}	9.87×10^{-13}
	6	1.03×10^{-17}	9.53×10^{-13}	9.89×10^{-13}
	7	4.83×10^{-13}	8.39×10^{-13}	10^{-12}
	8	1.63×10^{-13}	7.15×10^{-13}	9.95×10^{-13}
Testing	3	6.42×10^{-20}	9.71×10^{-14}	9.91×10^{-13}
	4	6.23×10^{-22}	5.01×10^{-13}	9.98×10^{-13}
	5	3.83×10^{-19}	8.76×10^{-14}	3.82×10^{-13}
	6	1.38×10^{-18}	7.35×10^{-13}	7.65×10^{-13}
	7	1.3×10^{-18}	9.94×10^{-13}	9.24×10^{-13}
	8	2.21×10^{-15}	7.77×10^{-13}	9.34×10^{-13}

[a] LM: levenberg–marquardt,
SCG: scaled conjugate gradient,
GDX: gradient descent with back propagation learning rate.
[b] MSE: mean square error.

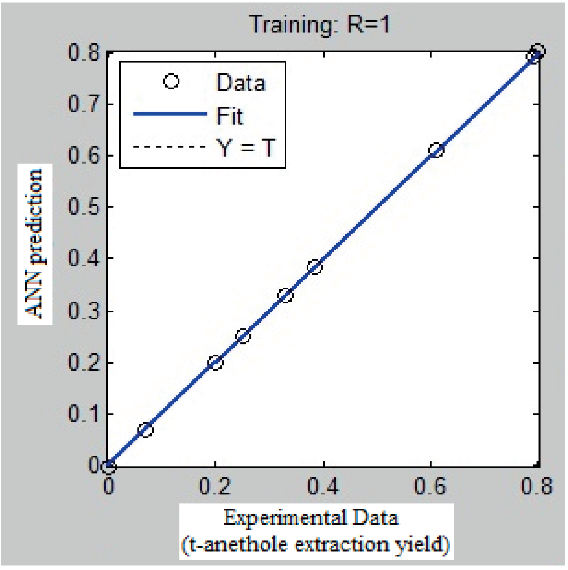

Fig. 2: Scatter plots of ANN modeling versus experimental data for training data.

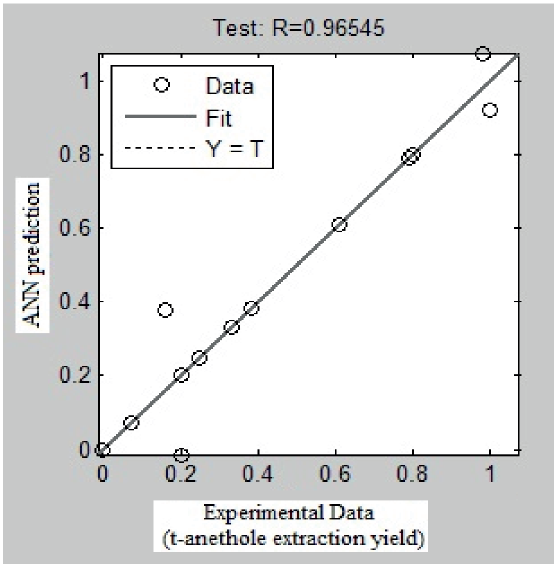

Fig. 3: Scatter plots of ANN modeling versus experimental data for testing data.

Fig. 2 shows information on the oil extraction yield by comparing the ANN model predicted values for training data against the experimental data. Fig. 3 indicates the simulated ones derived by ANN model for testing data which have not been applied for the training of the ANN (25% remaining data), for the extraction yield versus the experimental data. The correlation coefficient related with training data set is 1 and that for testing data set is 0.96. The figures show that the data obtained from the predicted model are in a very good agreement with the experimental results. The predictions that accordance measured values should be on the 45° line. Nearly all data are close to this line, which certifies the accuracy of the ANN model. The network weights and coefficients associated with this ANN model were calculated with the codes of a computer program written in MATLAB (version 2010a).

Also the LM training algorithm was found to have a preferable performance. SSE and epochs of training and testing for 4 neurons are shown in Table 3. The LM is the fastest training algorithm for moderate size networks and when the training set is large will occupy a small memory size [20].

Table 3. SSE and epochs of training and testing for the network with 5-nerouns.

Train algorithm [a]	Training		Testing		
	MSE[b]	R^2	MSE	R^2	Epochs
LM	1.7×10^{-18}	1	3.83×10^{-19}	0.965	23
SCG	5.62×10^{-13}	1	8.76×10^{-14}	0.60	221
GDX	9.87×10^{-13}	1	3.82×10^{-13}	0.445	2984

[a] LM: levenberg–marquardt,
SCG: scaled conjugate Gradient,
GDX: gradient descent with Back propagation learning rate.
[b] MSE: mean square error.

CONCLUSIONS

In this study, the t-anethole extraction yield via subcritical water technology was effectively modeled as a function of the independent variables (temperature, flow rate and mean particle size) by an optimal ANN. The optimal ANN was concluded to be the MLP network with five neurons in hidden layer and LM training algorithm. The predictive data of modeling algorithms are very suitable in contrast to experimental data. The optimal model was able to predict t-anethole yield with an error of 3.83×10^{-19}. So, it can be concluded that the ANN model characterized in optimum is an efficient tool to predict the extraction yield of essential oils by subcritical water extraction.

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