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ANN modeling of extraction kinetics of essential oil from tarragon using ultrasound pre-treatment

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ABSTRACT

In this paper, an artificial neural network (ANN) modeling is utilized to predict kinetics of essential oils extraction from tarragon (*Artemisia dracunculus* L.) using Ultrasound pre-treatment with Clevenger. A three-layer perceptron artificial neural network was created to predict the extract model with an error back-propagation algorithm. To design the ANN model, ultrasound power, sonication time, extraction time and their interactions were considered as input vectors while the extraction yield of essential oils was considered the model output. The performance of the network was optimized by varying the number of nodes in the hidden layer to achieve the best ANN architecture for output prediction. The performance of different ANN architectures was obtained as error (mean squared errors: MSE) and goodness of fit (determination coefficient: R^2) parameters. The results showed that the best prediction performance belonged to 3-7-1 ANN architecture (0.0008 normalized MSE and 0.99 R^2) which means that it is possible to predict the extraction yield of essential oils with an acceptable error having the three input parameters. The main extracted compounds by two methods at different conditions were estragole (76.6–83.0%), (Z)-β-ocimen (5.7–8.7%), (E)-β-ocimen (5.2–7.9%).

1. Introduction

There have been increasing interests toward essential oils (EOs) in several domains such as food engineering and pharmaceutical industries. They possess significant physicochemical properties and usually behave in an environment friendly manner. Therefore, they have extra values as being natural products. Because of their multi-biological activities, EOs are widely used in medicine. In fact, they show biocidal activities (bactericidal, virocidal and fungicidal) in immunology purposes. Their antimicrobial effects against multi-resistant bacteria have been proved by numerous studies (El Asbahani et al., 2015).

Tarragon (*Artemisia dracunculus* L.) is a herbaceous perennial plant in *Asteraceae* family. Two varieties of tarragon are known: French Tarragon and Russian Tarragon. Tarragon is a strong aromatic plant and is also considered as a medicinal plant (Arabhosseini et al., 2009). For example, tarragon extracts are useful for the treatment of wound healing, mouth diseases, kidney stone, toothache, burns, joint diseases, pulmonary tuberculosis, pneumonia and chronic bronchitis (Aglarova et al., 2008).

It is important that the most efficient extraction method used to achieve essential oils with high quality and efficiency. Hydro-distillation is the main and the most conventional method which is used for EOs extraction. However, hydro-distillation present some disadvantages: longer extraction time (3–6 h) which results in higher costs and can induce hydrolysis of some constituents of the essential oils such as esters by reaction with water at high temperatures to form acids and alcohols, difficulty to control the heat transfer in a constant manner all along the process, long term contact with boiling water leads to the hydrolysis of the terpene molecules and overheat and lose some polar molecules in water extraction, resulting in lower yields and losses of volatile compounds due to prolonged heating (Pingret et al., 2014; El Asbahani et al., 2015). Due to their significant properties, development of a suitable extraction method with maximum rate would be of critical importance. In this regard, selectivity of extraction processes has gained special interests. That's why, some adjustable parameters to control selectivity in conventional methods (e.g. hydro-distillation and solvent extraction) are still under study (Mitra et al., 2011).

Because of its cavitation property, ultrasound-assisted extraction (UAE) is considered a new technology which catalyzes heat and mass transfer. This technology is utilized massively in extraction applications (Chemat and Khan, 2011), including: extracting pectin from grape fruit peel (Wang et al., 2015), polysaccharides from blackcurrant (Xu et al., 2015), carvone and limonene from caraway seeds (Chemat et al., 2004).

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This UAE technique is very efficient due to several factors: it is very fast, consumes less fossil energy and also permits the reduction of solvents. Furthermore, it widens the selection ranges of the solvents and reinforces extraction efficiency (Vilkhu et al., 2008; Pingret et al., 2012). However, the effects of ultrasound on extraction yield and kinetics may be linked to the nature of the plant matrix (Wang and Weller, 2006). Thus, it is very ideal to offer various extraction techniques with higher efficiency and more powerful selectivity. There have been some studies relating to the extraction of essential oils by using different techniques of distillation and modern extraction methods, like ultrasound, microwave and supercritical fluid can be mentioned of course, the combined effect of using ultrasound and distillation an oil is considered, however, it's effect on the extraction efficiency is not regarded.

Due to their significantly and creditable properties in modeling complex relationships between variables, artificial neural networks (ANN) integrated with experimental design, have been used extensively during recent decades (Xi et al., 2013; Shojaeimehr et al., 2014). ANN uses interlinked mathematical nodes or neurons to build a network able to model complicated operational relationships (Sadrzadeh et al., 2008). Neural networks were invented in 1940s in order to assist cognitive scientists to understand the underlying behavior of nervous system. The learning process of human brain was the initial hint toward development of ANNs numerical structures. Therefore, they were developed and utilized as alternative mathematical tools for solving different problems occurring in the domain of system identification, prediction, pattern identification, classification, process control and so on. (Mjalli et al., 2007).

Dahmoune et al.(2015) used ANNs to investigate the functional parameters of UAE in the extraction of phenolic compounds from *P. lentiscus* leaves. The model was designed to assess the effects of process variables and their relationship toward reaching ideal conditions. Khajeh et al.(2012) studied the capability of a three-layer ANN model to foresee the extraction yield of essential oils from *Diplotaenia cachrydifolia* using supercritical fluid extraction. The input parameters of the model were pressure, temperature, extraction time and modifier volume. In another study, Kuvendziev et al.(2014) offered a three layer ANN for modeling and predicting the extraction yield of polyunsaturated fatty acids from lyophilized viscera matrixes. In their study, operating parameters were pressure, temperature, mass flow of CO_2 and extraction time. These factors were considered as the input vectors of the ANN, while extraction yield was an output vector.

The objective of this study was to investigate the possibility of using artificial neural network method to predict the kinetics model of tarragon essential oil extracted using water distillation with ultrasound pre-treatment. Operating values were considered ultrasound power, sonication time, extraction time and their interactions where extraction yield as an output vector.

2. Materials and methods

The raw material, tarragon was harvested from local farm of the Varamin, Iran, (35° 19′N, 51° 38′E). The tarragon leaves were cleaned and dried in the shadow and the dried leaves were separated from the stems and packed in plastic bags. The samples were stored at 4 °C prior to the experiments. Before any experiment, test samples were ground into powder for 30 s using an electric mill (320p, Pars Khazar, Iran).

2.1. Distillation

A Clevenger-type apparatus was used for hydro-distillation. Twenty grams (dry matter) of dried tarragon leaves was added to a flask and it was mixed with 500 ml of distilled water. The flask was then heated by heating mantle for 2 h counted from the time after condensation of the first drop of vapor in the acquisition column. The amount of oil was measured and afterwards the oil was collected. The oil was stored in glass vials in the refrigerator at 4 °C.

2.2. Ultrasound assisted extraction

In order to make ultrasound waves, an ultrasonic generator (AMMM-1000 W, MPI-ultrasonics, Switzerland) was used with production capacity of 1000 W and a frequency of 20 ± 5 kHz. The ultrasonic horn was used to generate and transmit ultrasonic waves in liquid media made of titanium with a diameter of 20 mm. Twenty grams (dry matter) of dried tarragon leaves was added to a beaker and it was mixed with 500 ml of distilled water. Ultrasound probe with 2 cm depth was placed in a beaker containing distilled water and samples. Samples were exposed to ultrasound at three sound power levels (250, 350 and 500 W) and three levels of sonication time (20, 30 and 40 min) with three replications. After sonication, the beaker's contents immediately transferred to Clevenger apparatus and extraction of these samples was done similar to what was explained in Section 2.1.

2.3. The kinetics of extraction

The oil content was recorded in the acquisition column with specified time intervals (2, 4, 6, 8, 10, 12, 15, 20, 40, 60, 80, 100 and 120 min) after observing the first drop in order to evaluate the kinetics of extraction. The amount of oil in the mentioned time was measured in ml by employing the conversion of column height to volume. With the conversion of column height to volume, the amount of oil in the mentioned time was reported in ml.

2.4. ANN modeling

A multi-layer perceptron ANN was developed to predict the extraction yield using Neural Network Toolbox. The network was trained with Levenberg – Marquardt Back propagation algorithm. Since the input parameters were extraction power, sonication time, and extraction time, the ANN architecture was a 3-*n*-1 network which represents three nodes in the input layer (ultrasonic power, sonication time and extraction time), *n* nodes in the hidden layer and one node in the output layer (extraction yield) (Fig. 1).

It is recommended to normalize the data along a correct spectrum to stop any numerical overflow during the training of an ANN. In this study, input and output parameters were normalized within a range of 0–1 using equation (1).

$$X_{norm} = \frac{X - X_{\min}}{X_{\max} - X_{\min}} \quad (1)$$

where X_{norm} is the normalized value, X is the actual value, and $X_{\max}$ and $X_{\min}$ are the maximum and minimum value, respectively.

The aim of normalizing the data is that the value of all elements in a template will be equivalent. Usually, input data to the neural network is scattered over a wide range. If no data is normalized during the training of the network, the effects of some parameters trained to the network may be underestimated or ignored. However, there are some

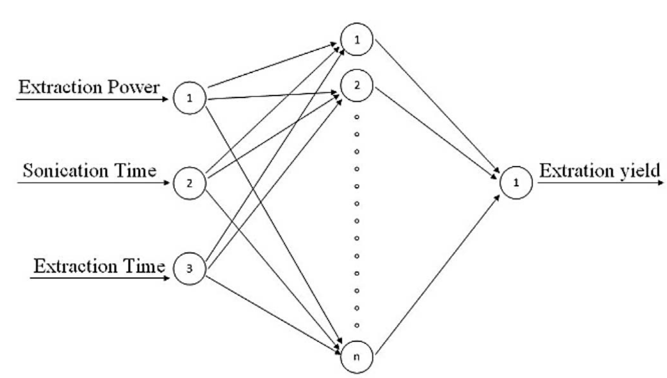

Fig. 1. ANN architecture.