Prediction of chamomile essential oil yield (*Matricaria chamomilla* L.) by physicochemical characteristics of soil

N. Khakipour 1(*), A. Mohammadi Torkashvand 2, A. Ahmadi 3, W. Weisany 2
1 Department of Soil Science, Savadkooh Branch, Islamic Azad University, Savadkooh, Iran.
2 Department of Horticulture, Science and Research Branch, Islamic Azad University, Tehran, Iran.
3 Department of Horticulture, University of Tabriz, Tabriz, Iran.

Key words: Artificial Neural Network (ANN), calcium carbonate equivalent (CCE), multilayer perceptron, nitrogen.

Abstract: The purpose of this study was to predict the percentage and yield of chamomile essential oils using the artificial neural network system based on some soil physicochemical properties. Several habitats of chamomile cultivation were investigated and 100 soil samples were shipped to the greenhouse. The maximum and minimum of pH, EC, K, OM (organic matter), CCE (calcium carbonate equivalent), and clay in soils were 8.75-7.94, 1.6-1.0, 381-135, 2.30-0.22, 69-16, and 55.6-32.0, respectively. Growth indices, essential oil percentage, and yield were measured. Artificial neural network modeling was carried out to predict the essential oil concentration and yield using three groups of soil properties as a predictor: 1- nitrogen (N), phosphorus (P), potassium (K), and clay; 2- pH, EC, organic matter (OM) and clay; 3- CCE, clay, silt, sand, N, P, K, OM, pH, and EC. So, three pedotransfer functions (PTFs) were developed using the multi-layer perceptron (MPL) with Levenberg-Marquardt training algorithm for estimating chamomile essential oil content. Results evaluation of the accuracy and reliability of showed that, the third PTF (PTF3) which developed by all independent variables had the highest accuracy and reliability. Results also showed that, it is possible to predict the concentration and yield of chamomile essential oil based on soil physicochemical properties. This issue is important in terms of land suitability, identify areas susceptible to chamomile cultivation and planning for essential oil yields.

1. Introduction

Optimum nutrition is a major condition for improving the quality and quantity of the crops, and it is affected by the soil environment (Barker and Pilbeam, 2007; Hargreaves et al., 2008; Ashoorzadeh et al., 2016; Ajili et al., 2018; Tofighi Alikhani, 2021). Peng et al. (2012) considered the role of soil characteristics to be highly effective in crops yield. Obviously, the production of organic materials in leaves without the presence of mineral...
elements in the process of photosynthesis is not possible. Each of the macronutrients plays a special role in the metabolism of plant growth. Bernier et al. (1981) concluded that flowering of plants was under the control of nutritional status, and in this regard, the balance between the elements that plant takes from air and soil is very important. Plant mineral compounds are one of the factors affecting the quality of crops (Prasad and Spiers, 1991).

Considering the importance of developing the cultivation of medicinal plants and using their products as natural ingredients compatible with human health, it is necessary to use different cultivation and nutrition methods that increase the essential oil and effective compounds of medicinal plants (Ajili et al., 2019; Savitikadi et al., 2020). Chamomile (Matricaria chamomilla L.) is an annual plant, aromatic, 20-40 cm high that grows wildly on fields and side roads (Omid Beigi, 2004). The plant now has a large dispersal in Europe, Western Asia, North Africa, North and South America, and Australia. The extensive cultivation of this plant is carried out in countries such as Hungary, Germany, Egypt, Czech Republic, Slovakia, and India (Omid Beigi, 2004). In Iran, different species of the genus Matricaria grow in different parts of the country. Chamomile flowers are used to treat stomach, flatulence, and skin lesions. In most western countries, they are used as appetizers and digestible foods. The active ingredient of chamomile has been mentioned for many medicinal properties such as sedative, anti-spasmodic, stimulating white blood cells and strengthening the body’s defense system, and antibacterial gram-positive and anti-allergic (Salamon, 1992). Accordingly, chamomile is used in many countries as dry flowers and essential oils in the pharmaceutical, food, cosmetic and sanitary industries. In recent years, it has also become one of the most popular pharmaceutical plants in the world (Gheedie Jashni et al., 2015). Upadhyay and Patra (2011) investigated the effects of calcium and magnesium on chamomile growth and yield and stated that the effect of magnesium on the growth and essential oil of chamomile was higher than that of calcium.

One of the main issues in producing agricultural and garden crops is a lack of ability to forecast production/yield using accessible and easily measured indicators (Mohammadi Torkashvand et al., 2020). Various factors affect the yield and essential oil content of the plant, including nutrition and physico-chemical properties of the soil (El-Gohary et al., 2015; Belal et al., 2016; Radkowski and Radkowska, 2018; Mohammadi Torkashvand et al., 2020). For example, it is hypothesized that one can estimate the yield of a product based on the concentration of nutrients in a leaf (Lahiji et al., 2018; Mohammadi Torkashvand et al., 2020), fruit (Mohammadi Torkashvand et al., 2019) or soil characteristics (Rahmani Khalili et al., 2020; Tashakori et al., 2020). In this case, it will be possible to plan fertilization or choosing the soil susceptible and suitable for planting, or the farmer has an estimate of his income and, accordingly, plans its costs for the future programs.

There are various predictive methods for estimating several natural variables, among which more transfer functions are used. Different regression methods have been widely used to derive transitional functions (Vereecen et al., 1992; Sepaskhah et al., 2000; Marashi et al., 2017; Esami et al., 2019). These methods consider the relationship between the input data and the data to be predicted to be predefined. Since the soil and plant are natural and heterogeneous systems, it is difficult to establish a connection between their properties. Therefore, in these systems, artificial neural networks (ANN) operate more efficiently than regression methods. Numerous studies have been carried out to estimate soil variables through artificial neural networks (Zhou et al., 2008; Bocco et al., 2010; Gago et al., 2010; Parvisi et al., 2010; Mokhtari Karchegani et al., 2011; Besalatpour et al., 2013; Dai et al., 2014; Moghimi et al., 2014; Aitkenhead et al., 2015; Marashi et al., 2017; Khanbabakhani et al., 2019; Marashi et al., 2019). Also, some studies have been conducted to predict crop yield by remote sensing, stochastic, artificial neural network (ANN) and simulation models (Bannayan and Crout, 1999; O’Neal et al., 2002; Bartoszek, 2014; Farjam et al., 2014; Dominguez et al., 2015; Emamgholizadeh et al., 2015; Dias and Sentelhas, 2017; Mohammadi Torkashvand et al., 2017; Niedbała, 2019; Mohammadi Torkashvand et al., 2019) based on weather, soil and growth characteristics as input data. Mohammadi Torkashvand et al. (2017) estimated the storage life of kiwifruit based on chemical characteristics of fruits, including the amount of nutrients by analyzing the neural network (NN), identifying it as a superior method in comparison to multiple regression. A similar study was carried out to predict kiwifruit yield based on leaf nutrients by ANN (Mohammadi Torkashvand et al., 2020). Tashakori et al. (2020) evaluated the efficiency of artificial neural network (ANN), multiple lin-
ear regression (MLR), and adaptive neuro-fuzzy inference system (ANFIS) in terms of saffron yield estimation by soil properties in some lands of Golestan province, Iran. According to the results, ANN showed the highest accuracy ($R^2= 0.58-0.89$) in estimating saffron yield as compared to MLR ($R^2= 0.41-0.47$) and ANFIS ($R^2= 0.41-0.69$) models.

Poorghadir et al. (2021) concluded that the yield and percentage of essence influenced by the soil properties and nutrition.

The purpose of this study was to investigate the importance of soil characteristics on the concentration and amount of chamomile essential oils and their estimation with respect to some important physicochemical properties of the soil, and investigation of feasibility of using artificial neural networks for estimating the concentration and amount of chamomile essential oils.

2. Materials and Methods

Soil experiments

Several habitats or areas of Chamomile cultivation were surveyed in Kermanshah and Hamadan provinces, West of Iran. From 20 areas, 100 soil samples (five of each area) were taken from soil depths of 0-30 cm and transferred to IAU, Science and Research Branch, Tehran, Iran. The environmental characteristics of the sampling areas, in particular the topographic and climatic characteristics, were similar. Soil samples were shipped to the laboratory and air-dried and clods were broken down in small particles with a plastic hammer; then they were passed through a sieve of 2 millimeters (Klute, 1986). Afterward, 0.5 kg of each soil was used for laboratory analysis and the rest was used for greenhouse experiments. The soil samples were analyzed for phosphorus, nitrogen and potassium nutrients, pH, Electrical Conductivity (EC), texture, and organic matter. Soil pH and EC were measured in saturated soil extract. Soil texture was determined by hydrometric method and the amount of calcium carbonate equivalent (CCE) was measured using titration method (Paye et al., 1948). The Kjeldahl method was used to measure nitrogen (Goos, 1995). Soil samples were extracted by Soltanpour and Schwab method (1977) and the concentration of available potassium and phosphorus were measured by flame emission and spectrophotometry methods (Emami, 1996). Organic matter was measured by Walkley and Black (1934) method. Some statistical data of soils are seen in Table 1.

**Greenhouse experiment**

In a completely randomized design, 100 different soil samples were sprayed in a plot (box) with dimensions of 30 to 35 cm and 25 cm in depth, and 20 seeds were planted in each plot. After germination and early growth of the plant, in the quadruple stage, the number of plants was reduced to 10 in each plot. During the growing season, field operations included irrigation, weed control and pest control for the plots were done alike for all the boxes.

After full flowering, the flowers were harvested at a maximum of five centimeters of length. The flowers were immediately dried at 60°C with an electronic dryer. In addition to the dry flower yield per plot in kg ha$^{-1}$, the concentration of essential oil for each soil was obtained. The essential oil content of the samples was determined by the Kelevenger apparatus by the water distillation method and expressed as g/100 g of dry flowers. The essential oil yield was expressed as kg/ha.

<table>
<thead>
<tr>
<th>Soil properties</th>
<th>pH</th>
<th>EC (dS/m)</th>
<th>N (%)</th>
<th>P (mg/kg)</th>
<th>K (mg/kg)</th>
<th>OM (%)</th>
<th>CCE (%)</th>
<th>Sand (%)</th>
<th>Silt (%)</th>
<th>Clay (%)</th>
<th>Essential oil (%)</th>
<th>Essential oil yield (kg/ha)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max</td>
<td>8.75</td>
<td>1.60</td>
<td>1.30</td>
<td>81.00</td>
<td>381.00</td>
<td>2.30</td>
<td>69.00</td>
<td>39.40</td>
<td>42.40</td>
<td>55.60</td>
<td>1.57</td>
<td>7.37</td>
</tr>
<tr>
<td>Min</td>
<td>7.94</td>
<td>1.00</td>
<td>0.25</td>
<td>8.00</td>
<td>135.00</td>
<td>0.22</td>
<td>16.00</td>
<td>14.50</td>
<td>21.00</td>
<td>32.00</td>
<td>0.01</td>
<td>0.28</td>
</tr>
<tr>
<td>Average</td>
<td>8.13</td>
<td>1.28</td>
<td>0.73</td>
<td>22.10</td>
<td>226.10</td>
<td>1.43</td>
<td>33.40</td>
<td>24.11</td>
<td>30.57</td>
<td>45.32</td>
<td>0.69</td>
<td>3.71</td>
</tr>
<tr>
<td>Median</td>
<td>8.06</td>
<td>1.25</td>
<td>0.78</td>
<td>16.50</td>
<td>244.00</td>
<td>1.46</td>
<td>28.50</td>
<td>23.20</td>
<td>30.25</td>
<td>46.75</td>
<td>0.76</td>
<td>4.13</td>
</tr>
<tr>
<td>Standard</td>
<td>0.22</td>
<td>0.15</td>
<td>0.37</td>
<td>18.93</td>
<td>62.28</td>
<td>0.50</td>
<td>13.83</td>
<td>5.69</td>
<td>4.80</td>
<td>6.16</td>
<td>0.51</td>
<td>2.61</td>
</tr>
<tr>
<td>Kurtosis</td>
<td>1.72</td>
<td>-0.61</td>
<td>-1.72</td>
<td>5.37</td>
<td>-0.70</td>
<td>0.34</td>
<td>-0.06</td>
<td>1.32</td>
<td>-0.30</td>
<td>-0.95</td>
<td>-1.23</td>
<td>-1.72</td>
</tr>
<tr>
<td>Skewness</td>
<td>1.67</td>
<td>0.15</td>
<td>0.02</td>
<td>2.61</td>
<td>0.28</td>
<td>-0.69</td>
<td>0.92</td>
<td>1.02</td>
<td>0.26</td>
<td>-0.38</td>
<td>0.26</td>
<td>-0.12</td>
</tr>
</tbody>
</table>

OM= Organic Matter; CCE= Calcium carbonate equivalent.
as kg ha⁻¹ in dry flower yield.

**Artificial neural network**

One of the best known rules is multilayer perceptron (MLP) learning rule. MLP is a feed forward network in which information flow from input side and pass through the hidden layers to the output layer to produce outputs. In this research, MLP rule and Levenberg-Marquart back propagation algorithm was used for training the artificial neural networks. The Tangent axon function was used as an activation function, which is a nonlinear function. Pourhaghi et al. (2013) also used the Tangent axon functions for predicting the input flows by ANN. NeuroSolutions 5.05 (NeuroDimension, Inc., Gainesville, FL, USA) software was used to design the artificial neural network.

The data used in training, validation and test were 60, 20 and 20% of the total data respectively. The training data are used for network education and training. Evaluation data are not used in network training, but this data are used to compare different models and to determine the most suitable network and PTFs.

The analysis of the neural network with three sub-series of variables as input variables was performed to estimate or predict the essential oil percentage and essential oil yield:

1 - In first step, total nitrogen, available phosphorus and potassium and clay content of soils, which are the most important factor in soil fertility, were selected as predictors and PTF1 was developed.

2 - In the second step, pH, EC, organic matter and clay, which are found in the most common and important measurements in standard soil analyses, were selected as predictors for estimation desired variables, and PTF2 was developed.

3 - In third step all of the measured soil properties (N, P, K, OM, CCE, pH, EC, Sand, Silt and Clay) were included as predictor for developing PTF3.

Therefore, three PTFs (PTF1, PTF2 and PTF3) were developed using ANNs and their efficiency was compared with each other to find the best and most suitable PTF.

The number of input layer nods was chosen as the number of input parameters for each desired issue. The number of hidden layers determines the complexity of the grid, and the reason for this complexity is that as the number of hidden layers increases, the number of connections between the verge layers increases, which leads to network complexity. The number of output layer neurons is equal to the number of output parameters of the desired problem.

After training the network with the data of the training and validation series, the precision and accuracy of the generated models were evaluated using the test series data.

In order to evaluate network accuracy, the coefficient of determination (R²) and square error squared (RMSE) were used.

\[
R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2} \quad (1)
\]

\[
RMSE = \sqrt{\frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{N}} \quad (2)
\]

In which: \(y_i, \bar{y}, \hat{y}\) respectively, the measured dependent variable, its mean and the estimated dependent variable, and N is the number of observations. Other criteria used to evaluate the precision of transition functions were the Geometric Mean Error Ratio (GMER) and Geometric Standard Deviation of error ratio (GSDER):

\[
GMER = \exp \left( \frac{1}{N} \sum_{i=1}^{N} \ln \left( \frac{\hat{y}_i}{y_i} \right) \right) \quad (3)
\]

\[
GSDER = \exp \left( \frac{1}{N - 1} \sum_{i=1}^{N} \left[ \ln \left( \frac{\hat{y}_i}{y_i} \right) - \ln(GMER) \right]^2 \right)^{1/2} \quad (4)
\]

Geometric mean of error ratio (GMER) represents the degree of conformance between measured and estimated values. If the GMER is equal to one, it represents a complete fit between measured and predicted values. If the GMER is greater than one, it indicates that the predicted values are greater than the measured values, and the GMER less than one is an indication of lower estimated values than the measured values. Geometric standard deviation of error ratio (GSDER) is a measure of data diffusion. If it is close to one, it shows less diffusion and the difference between one and the other represents the deviation of most estimates from the measured data.
### 3. Results and Discussion

**Correlation between variables**

Table 2 shows the correlation between the variables studied and the percentage and yield of the essential oils. The results presented in this table could be important to find input data series to the neural network. In our study, the percentage and yield of essential oil showed a positive and significant correlation with organic matter, N, P and K contents and clay. Jat and Ahaheat (2006) showed that the use of bio-fertilizers containing nitrogen, phosphorus and potassium increased the growth and amount of essential oil of the fennel plant. Phosphorus plays an important role in seed, flowers germination, vegetative growth, the acceleration of ripening and the completion of metabolic processes of fruits (Bennett, 1993; Malakouti and Shahabi, 2000; Malakouti et al., 2008). It is also involved in controlling enzymatic reactions and regulating metabolic pathways (Rejali, 2005; Miransari et al., 2007). Potassium affects the amount and quality of herbal essential oils due to its effect on metabolic pathways and enzymatic activity (Pacheco et al., 2008). In the case of potassium deficiency, the quality of some products, especially fruits and vegetables, decreases (Egilla et al., 2005; Mohiti et al., 2011). Potassium deficiency during plant growth leads to a decrease in photosynthetic rate and chlorophyll content (Geraldeaux et al., 2010), activation of enzymes, and reduced growth and yield (Kanai et al., 2007). Potassium interacts with almost all essential elements.

Furthermore, a synergistic role of K with either N or P has been already noted (Barker and Pilbeam, 2007). Nurzynska-Wierdak (2013), Cecilio Filho et al. (2015) and Chrysargyris et al. (2017 a) evaluated the impact of different potassium levels (275, 300, 325, 350 and 375 mg/L) on the morphological and biochemical characteristics of spearmint (*Mentha spicata* L.). The results showed that the potassium in 325 mg/L treatment could be appropriate for spearmint cultivation and production for essential oil uses. In the same study, Chrysargyris et al. (2017 b) found that the lavender grown in 300 mg L⁻¹ of K was appropriate for the essential oil uses/production while the 325 mg L⁻¹ of K were more appropriate for lavender cultivation for fresh and dry matter uses.

Due to the significant correlation of essential oils with organic matter, N, P and K contents and clay (Table 2), it was determined three series of data as input data of ANN that is observed in Table 3. Table 3 shows the number of hidden layers, and the number of nodes in the hidden layers in the three input series.

**Estimation (prediction) of essential oil**

Figure 1 shows the distribution of actual values (measured) and the estimation or prediction of the percentage of essential oil of chamomile and their conformity in three series of input data. $R^2$ was between the measured values and the estimated essential oils as observed in Table 4. As seen in the first transfer function (PTF1), $R^2$ was 82.71% in the test data and 78.56% in the training data series. The GMER value indicated that almost the network in the test data was not under or over-estimating, and its

<table>
<thead>
<tr>
<th>Variable</th>
<th>pH</th>
<th>EC</th>
<th>N</th>
<th>P</th>
<th>K</th>
<th>OM</th>
<th>CCE</th>
<th>Sand</th>
<th>Silt</th>
<th>Clay</th>
<th>Essential oil</th>
<th>Essential oil yield</th>
</tr>
</thead>
<tbody>
<tr>
<td>pH</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EC</td>
<td>0.511**</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>-0.101</td>
<td>0.152</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P</td>
<td>0.806**</td>
<td>0.546**</td>
<td>-0.382*</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>-0.390*</td>
<td>-0.419**</td>
<td>0.099</td>
<td>-0.323*</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>OM</td>
<td>0.414**</td>
<td>0.675**</td>
<td>0.362*</td>
<td>0.443**</td>
<td>-0.046</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CCE</td>
<td>-0.267</td>
<td>0.015</td>
<td>0.001</td>
<td>-0.287</td>
<td>0.044</td>
<td>-0.544**</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sand</td>
<td>-0.032</td>
<td>-0.339*</td>
<td>-0.439**</td>
<td>-0.029</td>
<td>0.268</td>
<td>-0.577**</td>
<td>0.648**</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Silt</td>
<td>-0.202</td>
<td>0.219</td>
<td>0.269</td>
<td>-0.069</td>
<td>-0.201</td>
<td>0.409**</td>
<td>-0.258</td>
<td>-0.408**</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Clay</td>
<td>0.188</td>
<td>0.178</td>
<td>0.243</td>
<td>0.084</td>
<td>-0.12</td>
<td>0.276</td>
<td>-0.465**</td>
<td>-0.711**</td>
<td>-0.353*</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Essential oil</td>
<td>0.092</td>
<td>-0.024</td>
<td>0.391*</td>
<td>0.278</td>
<td>0.434**</td>
<td>0.355*</td>
<td>-0.181</td>
<td>0.155</td>
<td>0.153</td>
<td>-0.277</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Essential oil yield</td>
<td>0.235</td>
<td>0.163</td>
<td>0.401*</td>
<td>0.423**</td>
<td>0.382*</td>
<td>0.449**</td>
<td>-0.101</td>
<td>0.226</td>
<td>0.246</td>
<td>-0.421**</td>
<td>0.919**</td>
<td>1</td>
</tr>
</tbody>
</table>
values were roughly one, but for the training data series the model overestimated. The $R^2$ value in the training data of the second series was 18.06% more than the first transfer function. In the test data, the $R^2$ value increased by 6.83%. The GMER value indicated that the model underestimated, and this is especially evident in the test data series.

According to the results of Table 4, when each of the nine variables was considered as inputs to the network, the distribution of estimated and measured values (Fig. 1) was reduced around the 1:1 axis and $R^2$ in training data is up to 96.62% and the test rose to 94.78%. Another important aspect is the more accurate estimation of the percentage of chamomile essential oil in both the training and test data, so that the GMER value in both data series was near one, indicating an accurate estimate and a lack or low estimate. The value of GSDER also showed that the lowest non-conformance of predicted essential oils with the measured values in the data of the training and test series in the third transfer function was observed. Based on these results, increasing variables from 4 (PTF1 model) to 9 (PTF3 model) decreased error and increased $R^2$ of ANN-model.

Mohammadi Torkashvand et al. (2020) employed an artificial neural network (ANN) to evaluate the kiwi yield of Hayward cultivar based on the concentration

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**Table 3** - Input data for constructing a neural network in three different transfer functions and the characteristics of neural networks made

<table>
<thead>
<tr>
<th>Transition function</th>
<th>Model inputs</th>
<th>No. of hidden layers</th>
<th>No. of hidden layer nodes 1</th>
<th>No. of hidden layer nodes 2</th>
<th>No. of hidden layer nodes 3</th>
<th>Type of transfer function</th>
<th>Type of target function</th>
</tr>
</thead>
<tbody>
<tr>
<td>PTF1</td>
<td>N, P, K and clay</td>
<td>3</td>
<td>4</td>
<td>2</td>
<td>1</td>
<td>Tangent axon</td>
<td>Levenberg-Marquardt algorithm</td>
</tr>
<tr>
<td>PTF2</td>
<td>pH, EC, Organic matter</td>
<td>3</td>
<td>4</td>
<td>4</td>
<td>2</td>
<td>Tangent axon</td>
<td>Levenberg-Marquardt algorithm</td>
</tr>
<tr>
<td>PTF3</td>
<td>All variables</td>
<td>1</td>
<td>10</td>
<td>-</td>
<td>-</td>
<td>Tangent axon</td>
<td>Levenberg-Marquardt algorithm</td>
</tr>
</tbody>
</table>

**Table 4** - Determination coefficient ($R^2$), error (RMSE), GMER and GSDER in two sets of training and test data in predicting essential oil concentration (g/100 g)

<table>
<thead>
<tr>
<th>Transition function</th>
<th>Data series</th>
<th>$R^2$</th>
<th>RMSE</th>
<th>GMER</th>
<th>GSDER</th>
</tr>
</thead>
<tbody>
<tr>
<td>PTF1</td>
<td>training</td>
<td>0.7856</td>
<td>0.226</td>
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<td>0.072</td>
<td>0.91</td>
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<td>1.57</td>
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<td>0.9478</td>
<td>0.086</td>
<td>1.02</td>
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</tbody>
</table>

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**Fig. 1** - Measured values (actual) and estimated concentration of essential oils in diagram 1: 1 test data and their conformance.
Khakipour et al. - Forecasting chamomile essential oil yield through soil physicochemical properties of nitrogen, potassium, calcium, and magnesium in leaves. They concluded that the maximum $R^2$ and the lowest root mean square error were obtained when all nutrients and related ratios were considered as input variables. Mohammadi Torkashvand et al. (2017) tested and compared the performance of an artificial neural network in predicting the firmness of six-month stored kiwifruit with different input datasets. Reversely, they showed that the best answer was obtained using ANN with a RMSE of 0.539 and a correlation coefficient of 0.850 ($R^2=0.724$) when the nitrogen and calcium (N/Ca ratio) were input data (two variables). Prediction of 6-month fruit firmness using nutrient concentrations and their ratios (8 variables) datasets resulted in the lowest $R$-value and the highest error (Mohammadi Torkashvand et al., 2017).

Figure 2 shows the dispersion of the measured yield values and the estimation of essential oil in the test series in chart 1:1 and in the 20 samples. According to the results of Table 5, the value of $R^2$ in the test data series in the first transfer function was 91.25%, but less than 80% in the training data. The other thing is the high amount of dispersion, non-conformance of the estimated and measured and over-estimation data in training. Therefore, in the test series, the accuracy has increased, and in addition to reducing the dispersion and increasing the conformance, the prediction accuracy has significantly increased, because GMER was approximately one. Forecasting models of plant yield are prognostic tools that can be an important element in precision agriculture (Shearer et al., 2000; Dias and Sentelhas, 2017; Prasad et al., 2017; Mohammadi Torkashvand et al., 2017, 2020) and the principal factor in decision-making systems (Park et al., 2005). Akbar et al. (2018) used a model based on artificial neural network to predict essential oil yield in turmeric (Curcuma longa L.). The data of essential oil, soil and environmental factors were collected from 131 turmeric germplasms in 8 agro-climatic regions of Odisha. Results showed that multilayer-feed-forward neural networks was the most reasonable model to use with $R^2$ value of 0.88. Niazhian et al. (2018) calculated a root mean square error (RMSE) of 0.192 and $R^2$ of 0.901 in predicting essential oil content of Ajowan by using the artificial neural network when the number of rays, pedicels, and flowers per umbellet, and a number of umbellets in an umbel, inputted variables. Bahmani et al. (2018) utilized an artificial neural network modeling to predict kinetics of essential oils extraction from tarragon (Artemisia dracunculus L.) using ultrasound pre-treatment with Clevenger. Based on results, the best prediction performance was belonged to 3-7-1 ANN architecture (0.0008 normalized mean squared error and $R^2$ were respectively 0.0008 and 0.99) which means that it is possible to predict the extraction yield of essential oils with an acceptable precision. Tashakori et al. (2020) research showed that a model with organic matter, phosphorus, potassium, and calcium carbonate as in dependent variables, was the best model ($R^2 = 0.87$) in estimating saffron yield.

If the focus is on the test data, in the second transfer function, the accuracy of the model ($R^2 = 83.23\%$) was less than the other two functions and its accuracy is much lower than the other two, so that the deviation of the measured and estimated essential oil yield data was 1.45 (GSDER) and the model had an over-estimation of 26% (GMER=1.26). The important point is that, like the content of essential oil (g/100 g dry matter), the highest accuracy and precision of the neural network model was obtained in predicting the essential oil yield in the third transfer function.
fer function, in which all soil variables (nine variables) were considered as input variables of the network. In the test data series, the lowest error (RMSE = 0.088) and the most consistent measured and estimated data on the essential oil yield were obtained in the third transfer function, although the fitted model had a lower estimation than the first function. Of course, it should be noted that in view of the great difference between the first and third functions in training data, the third function had a higher credibility in general.

4. Conclusions

In general, according to the results, the third transfer function (9 variables as input variables of the network) was the most accurate for estimation of the essential oil concentration and for the estimation of essential oil yields. They had the highest R² and the lowest RMSE values. Also, the estimated values of these functions were the most consistent with the observed values and the least deviation from the 1:1 line. As the R², RMSE, GMER and GSDER values of the proposed model for estimating essential oil percent for test series data were 94.78, 0.86, 1.02 and 1.32, respectively, and to evaluate the essential oil yield in the test series data respectively, equal to 91.51, 0.608, 0.92 and 1.20 respectively. Therefore, the results showed that with high accuracy and precision, it is possible to predict the concentration and yield of chamomile essential oil based on soil physicochemical properties. This issue is important in terms of land suitability, making possible to identify areas susceptible to chamomile cultivation and to plan for essential oil yields. It is suggested to model the prediction of the percentage and yield of chamomile essential oil with an artificial neural network with other characteristics of the soil alone or in combination with these characteristics and compare the results. It is also suggested that other models, such as neuro fuzzy should be evaluated for estimating the concentration and essential oil of chamomile as well as other medicinal plant species.

References


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