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Research Article
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Expectation of Chamomile Fundamental Oil Abdicate by Using the Artificial Neural Network System

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Abstract

The aim of this research was to forecast the proportion and production of chamomile essential oils by employing an artificial neural network system reliant on specific soil physicochemical characteristics. Various chamomile cultivation sites were explored, and 100 soil samples were transported to the greenhouse. The pH, EC, K, OM (organic matter), CCE (calcium carbonate equivalent), and clay content in the soils ranged from 8.75 to 7.94, 1.6 to 1.0, 381 to 135, 2.30 to 0.22, 69 to 16, and 55.6 to 32.0, respectively. Growth parameters, essential oil percentage, and yield were measured. The artificial neural network modeling aimed to predict essential oil concentration and yield using three sets of soil properties as predictors: 1- lime, clay, pH and EC; 2- nitrogen, phosphorus, potassium and clay; 3- lime, clay, silt, gravel, nitrogen, phosphorus, potassium, pH and EC. Consequently, three pedotransfer functions (PTFs) were formulated using the multi-layer perceptron (MLP) with the Levenberg-Marquardt training algorithm to estimate chamomile essential oil content. The evaluation of results indicated that the third PTF (PTF3), developed using all independent variables, exhibited the highest accuracy and reliability. Furthermore, the findings suggested the feasibility of predicting chamomile essential oil concentration and yield based on soil physicochemical properties. This has significant implications for land suitability assessments, identifying areas conducive to chamomile cultivation, and planning for essential oil yields.

Keywords: Artificial neural network (ANN), Calcium carbonate equivalent (CCE), Multilayer perceptron, Nitrogen.

INTRODUCTION

Ensuring optimal nutrition is a crucial factor in enhancing both the quality and quantity of crops, a condition profoundly impacted by the soil environment (Ajili Lahiji *et al*., 2018; Tofighi Alikhani, 2021). The role of soil characteristics in influencing crop yield has been emphasized by Peng *et al*. (2012), highlighting the indispensability of mineral elements in the process of photosynthesis for the production of organic materials in leaves. Each macronutrient plays a distinct role in the metabolic processes governing plant growth (Benier *et al*., 1985). The nutritional status, particularly the balance between elements extracted from air and soil, significantly influences plant flowering.

Given the significance of advancing the cultivation of medicinal plants and harnessing their products as natural, health-compatible ingredients, employing diverse cultivation and nutrition methods is essential to augment the essential oil and active compound content of medicinal plants (Ajili Lahiji *et al*., 2018; Savitikadi *et al*., 2020). Chamomile is an annual or perennial plant belonging to the Asteraceae family. The plant improves appetite and reduces swelling, pain and sweating (Ubessi *et al*., 2019). Chamomile are native to temperate regions of Asia and Europe and are grown around the world for their high medicinal, cosmetic, and dietary values (Wan *et al*., 2019). It has been used for thousands of years in ancient Greece, Rome and Egypt. In China, the detailed uses of this plant were first recorded in Uyghur medicine. Experienced TCM practitioners believe that preparations containing chamomile have a soothing effect. Additionally, the plant is used in traditional, homeopathic and Unani preparations (Zhao *et al*., 2015). There are two main varieties of chamomile: *Matricaria chamomilia* L. and *Anthemis nobilis* (L.). *Matricaria chamomilia* L. belongs to the genus Matricaria. This is an annual plant and the flowering period is from May to July in China. *Chamaemelum nobile* L. is a perennial plant of the genus Chamaemelum. The flowering period is from April to May in China (Dai *et al*., 2022). *Matricaria chamomilia* L. is relatively common and has been the subject of much research and use. Currently, 26 countries around the world have included this plant in their pharmacopoeia. Chamomile heads are often used as medicine (Petronilho *et al*., 2011). Chamomile contains flavonoids, coumarins, volatile oils, terpenes, sterols, organic acids and polysaccharides, among other compounds. Possessing a wide range of compounds, chamomile has various pharmacological activities such as anti-cancer, anti-infectious, anti-inflammatory, anti-oxidant, hypoglycemic, hypotensive, hypolipidemic, anti-allergic, anti-depressant and neuroprotective, among many other effects (Zhao, 2018). In general, this plant has special research value. However, there is little criticism on this topic in the literature. This article provides a comprehensive overview of plant properties and distribution, traditional uses, chemical composition, pharmacological effects, and quality control methods of chamomile (Dai *et al*., 2022).

Notably, the growth and essential oil yield of chamomile are influenced by factors such as calcium and magnesium, with magnesium exhibiting a more significant impact than calcium (Upadhyay and Patra, 2011). In the realm of agriculture, a key challenge lies in predicting crop yield based on readily accessible indicators. Various factors, including soil nutrition and physicochemical properties, affect plant yield and essential oil content (Belal *et al*., 2016; Radkowski and Radkowska, 2018; Mohammadi Torkashvand *et al*., 2020). Hypotheses suggest that predicting yield is feasible by assessing nutrient concentrations in leaves (Ajili Lahiji *et al*., 2018; Mohammadi Torkashvand *et al*., 2020), fruits (Mohammadi Torkashvand *et al*., 2019), or soil characteristics (Rahmani Khalili *et al*., 2020; Tashakori *et al*., 2020). Such predictions enable effective planning for fertilization, soil selection, and future financial considerations for farmers.

In predicting natural variables, transfer functions, especially artificial neural networks (ANN), have proven more efficient in heterogeneous natural systems like soil and plants compared to traditional regression methods. Numerous studies have successfully employed ANN to estimate soil variables and predict crop yield based on factors such as weather, soil properties, and growth characteristics (Zhou *et al*., 2008; Bocco *et al*., 2010; Mokhtari Karchegani *et al*., 2011; Besalatpour *et al*., 2013; Dai *et al*., 2014; Moghimi *et al*., 2014; Marashi *et al*., 2017; Marashi *et al*., 2019). Tashakori *et al*. (2020) specifically highlighted the superior accuracy of ANN in estimating saffron yield compared to multiple linear regression and adaptive neuro-fuzzy inference system models.

A study by Poorghadir *et al*. (2021) underscored the influence of soil properties and nutrition on the yield and essence percentage of crops. This study aims to delve into the impact of soil characteristics on the concentration and quantity of chamomile essential oils, exploring the feasibility of using artificial neural networks to estimate these essential oil parameters based on critical physicochemical soil properties.

MATERIALS AND METHODS

Soil experiments

Multiple locations for chamomile cultivation in Kermanshah and Hamadan provinces, West of Iran, were investigated. From 20 areas, a total of 100 soil samples (five from each area) were collected at a depth of 0-30 cm and sent to IAU, Science and Research Branch, Tehran, Iran. The sampling areas shared similar topographic and climatic characteristics. Soil samples underwent air-drying, and clods were fragmented into small particles using a plastic hammer before passing through a 2 mm sieve (Klute, 1986). Laboratory analyses, focusing on phosphorus, nitrogen, potassium nutrients, pH, electrical conductivity (EC), texture, and organic matter, were conducted using 0.5 kg of each soil sample. The remaining soil was dedicated to greenhouse experiments. Soil pH and EC were measured in saturated soil extracts, soil texture was determined hydrometrically, and calcium carbonate equivalent (CCE) was assessed through titration (Paye *et al*., 1948). Nitrogen was measured via the Kjeldahl method (Goos, 1995), and available potassium and phosphorus concentrations were determined by flame emission and spectrophotometry methods after soil extraction (Soltanpour and Schwab, 1977; Emami, 1996). Organic matter content was determined by the Walkley and Black method (1934). Statistical data regarding soil properties are presented in table 1.

Greenhouse experiment

In a completely randomized design, 100 distinct soil samples were applied to plots with dimensions of 30 by 35 cm and a depth of 25 cm, with 20 seeds planted in each plot. Following germination and early growth, the number of plants per plot was reduced to 10 during the quadruple stage. Standard field operations, including irrigation, weed control, and pest management, were uniform across all plots. Upon full flowering, flowers were harvested at a maximum length of five centimeters, dried at 60 ºC, and the dry flower yield per plot (kg ha^{-1}) and essential oil concentration were determined. Essential oil content was measured using the Clevenger apparatus and expressed as g/100 g of dry flowers, while essential oil yield was reported as kg ha^{-1} based on dry flower yield.

Artificial neural network

The multilayer perceptron (MLP) learning rule, a feedforward network, was employed in this study. The Levenberg-Marquart back propagation algorithm facilitated training, utilizing the Tangent axon function as the activation function. The design of the artificial neural network was executed using NeuroSolutions 5.05 software. Data were divided into training (60%), validation (20%), and test (20%) sets. Three sub-series of variables were used as input variables for estimating essential oil percentage and yield. The efficiency of three pedotransfer functions (PTF1, PTF2, and PTF3) was compared, each developed using different sets of predictors. The evaluation criteria included the coefficient of determination (R^2) and root mean square error (RMSE). The number of neurons in the input layer corresponded to the input parameters, while the complexity of the network was determined by the number of hidden layers. The output layer neurons matched the number of output parameters. Model precision and accuracy were assessed using the test set data after training with the training and validation set data.

$$R^2 = 1 - \frac{\sum_1^N (y_i - \hat{y}_i)}{\sum_1^N (y_i - \bar{y}_i)^2}$$

$$RMSE = \sqrt{\frac{\sum_1^N (y_i - \hat{y}_i)^2}{N}}$$

In which: yi, $\bar{y}$, $\hat{y}$ 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):

$$\mathrm{GMER} = \exp\left(\frac{1}{\mathrm{N}} \sum_{1}^{\mathrm{N}} \ln\left(\frac{\hat{\mathrm{Y}}_{\mathrm{i}}}{\mathrm{Y}_{\mathrm{i}}}\right)\right)$$

$$\mathrm{GSDER} = \exp\left(\frac{1}{\mathrm{N}-1} \sum_{i=1}^{N} \left[\ln\left(\frac{\hat{Y}_i}{Y_i}\right) - \ln(\mathrm{GMER})\right]^2\right)^{1/2}$$

The Geometric Mean of Error Ratio (GMER) serves as an indicator of the level of agreement between measured and estimated values. A GMER equal to one signifies a complete alignment between measured and predicted values. A GMER greater than one suggests that the predicted values surpass the measured values, while a GMER less than one indicates that the estimated values are lower than the measured values. On the other hand, the Geometric Standard Deviation of Error Ratio (GSDER) functions as a measure of data dispersion. A value close to one indicates minimal dispersion, and the deviation from one reflects the extent to which most estimates deviate from the measured data.

RESULTS AND DISCUSSION

Table 1 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. As seen, the percentage and yield of essential oil with organic matter showed a positive and significant correlation.

Table 1. Correlation between the input variables of the neural network and the amount of essential oil and essential oil yield.

Variable	pH	EC	N	P	K	OM	Lime	Sand	Silt	Clay	Essential oil	Essential oil yield
pH	1											
EC	0.511**	1										
N	-0.101	0.152	1									
P	0.806**	0.546**	-0.382*	1								
K	-0.390*	-0.419**	0.099	-0.323*	1							
OM	0.414**	0.675**	0.362*	0.443**	-0.046	1						
Lime	-0.267	0.015	0.001	-0.287	0.044	-0.544**	1					
Sand	-0.032	-0.339*	-0.439**	-0.029	0.268	-0.577**	0.648**	1				
Silt	-0.202	0.219	0.269	-0.069	-0.201	0.409**	-0.258	-0.408**	1			
Clay	0.188	0.178	0.243	0.084	-0.12	0.276	-.465**	-0.711**	-0.353*	1		
Essential oil	0.092	-0.024	0.391*	0.278	0.434**	0.355*	-0.181	0.155	0.153	-0.277	1	
Essential oil yield	0.235	0.163	0.401*	0.423**	0.382*	0.449**	-0.101	0.226	0.246	-0.421**	0.919**	1

*and **: Significant at P < 0.05 and P < 0.01, respectively.

Correlation among variables

The correlation between the variables examined and the percentage and yield of essential oils is depicted in table 2, offering valuable insights into potential input data for the neural network. Our findings reveal a positive and significant correlation between the percentage and yield of essential oil with organic matter, N, P, K contents, and clay. Consistent with our results, Jat and Ahaheat (2006) demonstrated that bio-fertilizers containing nitrogen, phosphorus, and potassium enhance the growth and essential oil production of fennel plants. Phosphorus plays a pivotal role in seed and flower germination, vegetative growth, fruit maturation, and metabolic processes (Bennett, 1993; Malakouti and Shahabi, 2000; Malakouti *et al*., 2008). Additionally, potassium influences herbal essential oil quantity and quality by affecting metabolic pathways and enzymatic activity (Pacheco *et al*., 2008). The correlation findings align with previous studies emphasizing the role of these elements in enhancing essential oil production (Nurzynska-Wierdak, 2013; Cecílio Filho *et al*., 2015; Chrysargyris *et al*., 2017).

Table 2. Input data for constructing a neural network in three different transfer functions and the characteristics of neural networks made.

Transition function	Model inputs	Number of hidden layers no.	Number of hidden layer nodes 1	Number of hidden layer nodes 2	Number of hidden layer nodes 3	Type of transfer function	Type of target function
PTF1	N, P, K and clay	3	4	2	1	Tangent axon	Levenberg-Marquardt algorithm
PTF2	pH, EC, Organic matter and clay	3	4	4	2	Tangent axon	Levenberg-Marquardt algorithm
PTF3	All variables	1	10	-	-	Tangent axon	Levenberg-Marquardt algorithm

Given the significant correlation with essential oils, three data series were designated as input for the artificial neural network (ANN), as outlined in table 3, considering the number of hidden layers and nodes.

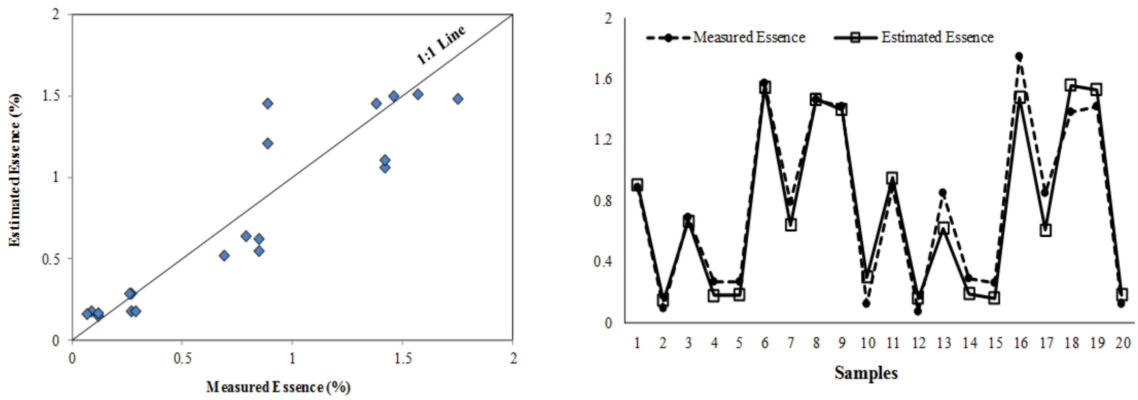
Table 3. Determination coefficient (R2), error (RMSE), GMER and GSDER in two sets of training and test data in predicting essential oil concentration (g/100 g).

Transition function	Data series	R^2	RMSE	GMER	GSDER
PTF1	Training	0.7856	0.226	1.27	2.37
	test	0.8271	0.201	1.04	1.24
PTF2	Training	0.9662	0.072	0.91	2.27
	test	0.8954	0.237	0.83	1.57
PTF3	Training	0.9562	0.023	0.98	1.22
	test	0.9478	0.086	1.02	1.32

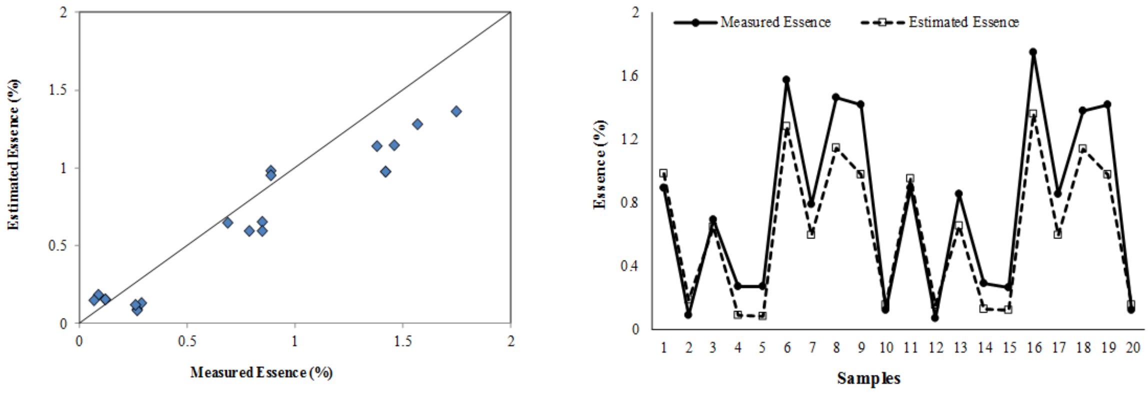
Estimation of essential oil

Fig. 1 illustrates the distribution and alignment of actual (measured) and estimated essential oil percentages for three input data series. R^2 values, as presented in table 4, indicate the accuracy of the ANN models in predicting essential oil percentages. Notably, the inclusion of all nine variables in the third transfer function (PTF3) resulted in a higher accuracy (R^2)

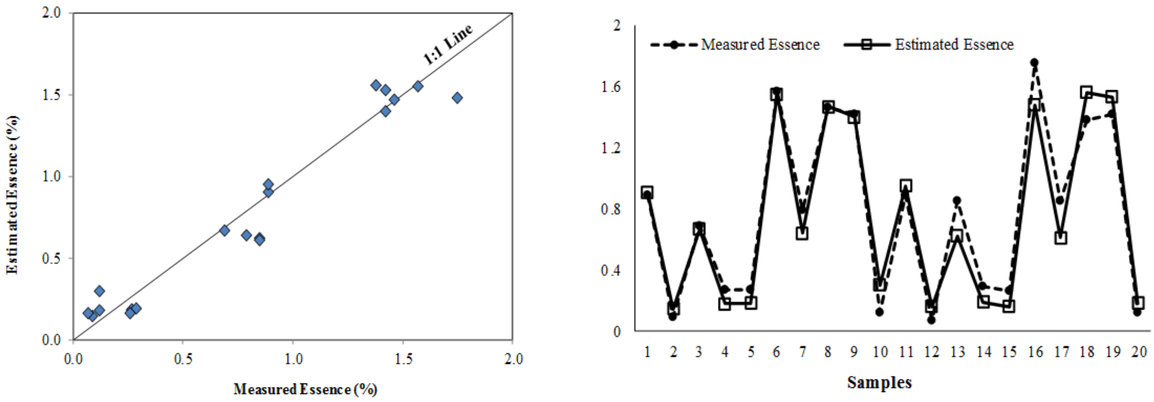
in both training (96.62%) and test (94.78%) data sets compared to PTF1 and PTF2. This increase in variables led to a reduction in error, as indicated by the GMER and GSDER values, demonstrating improved precision in the estimation of chamomile essential oil percentage.



A) First dataset



B) Second dataset



C) Third dataset

Fig. 1. Measured values (actual) and estimated concentration of essential oils in diagram 1: 1 test data and their conformance.

Table 4. Determination coefficients (R2), error (RMSE), GMER and GSDER in two sets of training and test data to predict the essential oil yield (kg / ha).

Transition function	Data series	R^2	RMSE	GMER	GSDER
PTF1	Training	0.7984	1.27	1.47	2.16
	test	0.9125	0.670	1.01	1.25
PTF2	Training	0.8646	0.536	1.19	1.38
	test	0.8323	0.998	1.26	1.45
PTF3	Training	0.9654	0.088	0.98	1.10
	test	0.9251	0.608	0.92	1.20

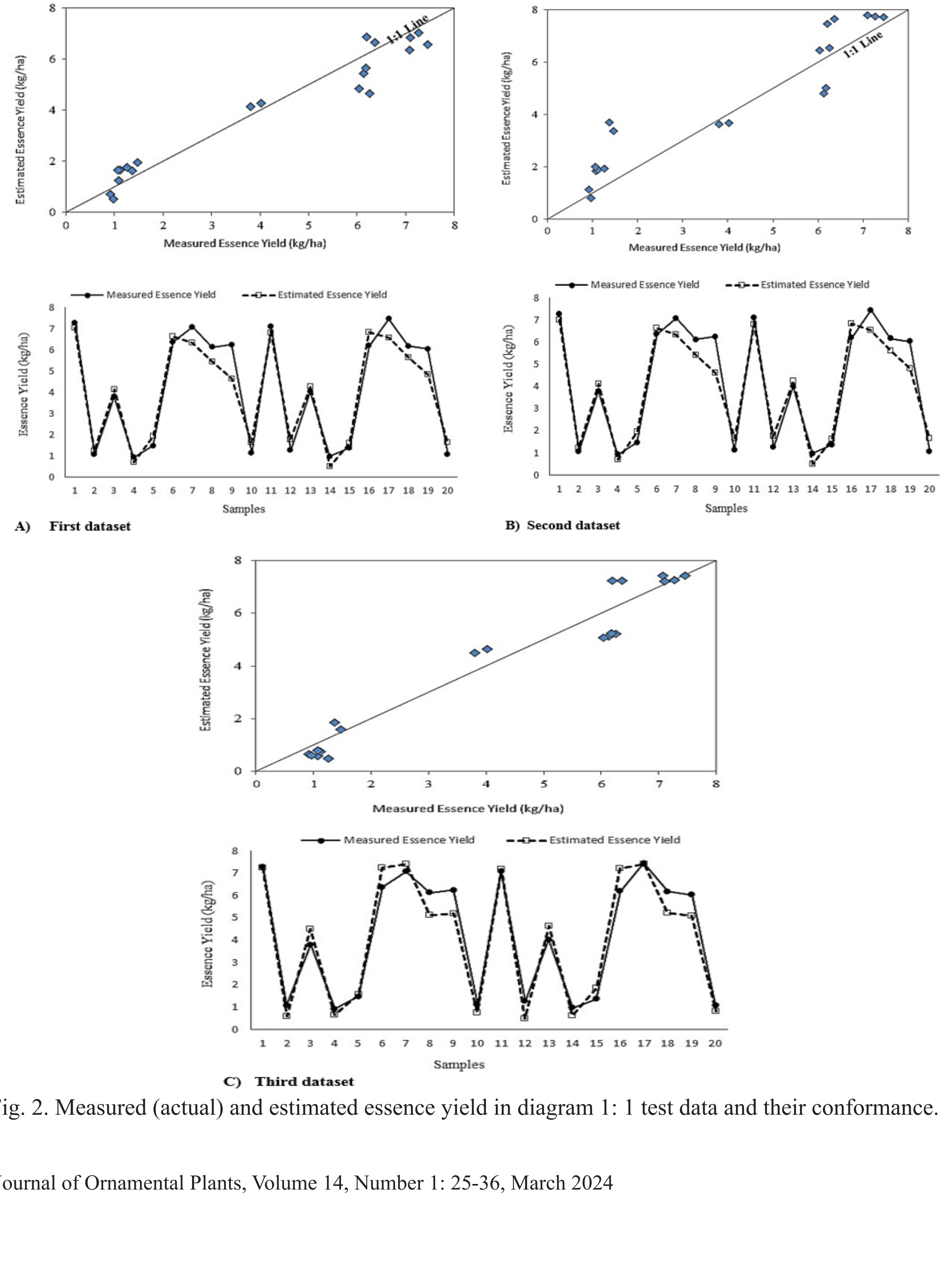


Fig. 2. Measured (actual) and estimated essence yield in diagram 1: 1 test data and their conformance.

Similarly, Fig. 2 displays the dispersion of measured yield values and the estimated essential oil values for the test series. The accuracy of the model improved in the third transfer function (PTF3), with an R^2 of 91.25% in the test data set. Despite a lower estimation in PTF3, the model exhibited the least error, as indicated by the GMER and GSDER values, demonstrating enhanced accuracy in predicting chamomile essential oil yield.

These results align with findings from studies employing ANN for crop yield prediction, emphasizing the importance of considering multiple variables for improved accuracy (Mohammadi Torkashvand *et al*., 2017; Akbar *et al*., 2018; Niazian *et al*., 2018). In summary, the comprehensive consideration of all nine soil variables led to a more accurate and reliable estimation of chamomile essential oil content and yield, showcasing the potential of ANN models in precision agriculture and decision-making systems.

CONCLUSION

In summary, the findings indicate that the third transfer function, incorporating nine variables as input for the neural network, proved to be the most precise in estimating both the concentration and yield of essential oil. This function exhibited the highest R^2 values and the lowest RMSE values, showcasing superior accuracy. Furthermore, the estimated values from this function demonstrated the closest alignment with observed values, displaying minimal deviation from the 1:1 line. The proposed model's evaluation metrics for estimating essential oil percentage in the test series data were as follows: R^2 = 94.78, RMSE = 0.86, GMER = 1.02, and GSDER = 1.32. Similarly, for essential oil yield in the test series data, the metrics were R^2 = 91.51, RMSE = 0.608, GMER = 0.92, and GSDER = 1.20. These results affirm the high accuracy and precision of predicting chamomile essential oil concentration and yield based on soil physicochemical properties. This predictive capability holds significance in determining land suitability, allowing for the identification of areas conducive to chamomile cultivation and facilitating strategic planning for essential oil yields. Future research avenues could explore additional soil characteristics or combinations thereof in conjunction with artificial neural networks for chamomile essential oil prediction. Additionally, the evaluation of alternative models, such as neuro-fuzzy, warrants consideration for estimating the concentration and essential oil yields not only for chamomile but also for other medicinal plant species.

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Conflict of Interest: The authors declare that they have no conflict of interest.

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