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Prediction of soil potassium forms using physicochemical properties and exchangeable potassium: I. Artificial neural network modeling

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ABSTRACT

Accurate prediction of soil potassium (K) fractions is critical for advancing precision nutrient management and promoting agricultural sustainability. This study aimed to develop artificial neural networks (ANNs) to predict multiple K fractions, including water-soluble, available (water-soluble + exchangeable), non-exchangeable, and total K prior to K amendment, and water-soluble, exchangeable, and fixed K following K amendment. Predictions were made using soil physicochemical properties such as clay, silt, sand, pH, organic carbon, cation exchange capacity, and electrical conductivity, along with measured exchangeable K and fertilizer-derived K. A comprehensive dataset, curated from peer-reviewed studies encompassing diverse global soils, served as the foundation for ANN development, ensuring broad applicability across different soil types and agroecological conditions. Multilayer perceptron ANNs with varying architectures were systematically optimized in MATLAB software, yielding high-fidelity models with robust predictive performance (correlation coefficients: 0.91–0.99). The complexity of the ANNs was tailored to the chemical dynamics of each K fraction. Simple architectures (8-8-1) effectively captured the distributions of water-soluble and fixed K, while more intricate configurations (8-10-10-10-1) were requisite for accurately modeling total K due to its complex interactions with soil matrices. Model validation confirmed high accuracy and reliability, with minimal mean squared error across all predicted fractions. To bridge the gap between research and practical application, these ANNs were embedded into an open-source, Excel-based tool, enabling seamless prediction of K fractions through user-friendly inputs of soil properties and measured exchangeable K data. This tool empowers farmers, agronomists, and researchers to optimize K fertilization strategies, reduce nutrient waste, and enhance crop productivity. The tool is accessible for download at: https://drive.shahroodut.ac.ir/index.php/s/fayE0zUH16TQe2M

Keywords: Excel-based tool, potassium fraction, precision agriculture, soil fertility.

1. Introduction

Potassium (K) is an essential macronutrient that plays a pivotal role in numerous physiological and biochemical processes in plants, including enzymatic activation, carbon and nitrogen metabolism, sugar translocation, protein synthesis, and photosynthetic efficiency (Xu et al., 2020). In the context of precision agriculture, maintaining optimal K levels is crucial because even slight imbalances can disrupt the uptake of other key nutrients, such as magnesium (Tränkner et al., 2018), calcium, sodium, and nitrogen (Du et al., 2017; Hu et al., 2017), and ultimately compromise crop productivity. The bioavailability of K in soil is regulated by a complex equilibrium among water-soluble, exchangeable, non-exchangeable, and structural pools, with each fraction governed by soil physicochemical attributes such as mineralogy, cation exchange capacity (CEC), texture, and organic carbon (OC) (Najafi-Ghiri and Abtahi, 2013).

Despite decades of research, the mechanisms governing K dynamics remain poorly characterized because of the nonlinear interactions between soil physicochemical properties and K fractions. Conventional statistical methodologies, such as correlation analyses and multiple linear regression (MLR) have been widely used to assess relationships among K pools and soil attributes. However, the weak to moderate correlation coefficients (r= 0.44-0.47) commonly reported highlight the inability of these linear approaches to capture the nonlinear and multifactorial interactions governing K dynamics (e.g., Najafi-Ghiri and Abtahi, 2013). Although subsequent studies employing MLR and path coefficient analysis (Wang et al., 2006; Zornoza et al., 2007) have sought to enhance predictive accuracy, the inherent assumption of linearity in these models limits their capacity to describe the complex and often nonlinear behavior of soil nutrient systems (Faraway, 2016). As a result, there remains a critical need for more sophisticated and flexible modeling frameworks capable of handling multivariate, nonlinear, and independent relationships among soil physicochemical variables. Developing such predictive tools is essential not only for advancing the theoretical understanding of soil K dynamics but also for improving site-specific fertilizer recommendations and reducing the environmental risks associated with nutrient over-application.

Table 1. Summary of soil samples and locations used in ANN analysis.

Location and number of sites	Soil depth for sample collection	Reference
15 sites in El-Dakhla soils, Egypt	0-30, 30-60 cm	Awad et al. (2016)
20 sites in Haveri district, Karnataka, India	0-20, 20-50 cm,	Harsha and Jagadeesh (2017)
14 sites in Fars Province, Iran	0-20 cm	Sadri et al. (2016)
6 sites in Kohgiluyeh and Boyer-Ahmad Province, Iran	Various horizons (3–4 layers)	Shakeri and Abtahi (2019)
10 sites in Homs, Syria	0-20 cm	Shamsham et al. (2019)
9 sites in tobacco-growing soils of Gilan, Mazandaran, and Golestan Provinces, Iran	Various horizons (5–7 layers)	Gholizadeh et al. (2016)
9 sites distributed across various regions from northern to southern Portugal	0-20, 20-50, 15-35 cm	Portela et al. (2019)
16 sites distributed across northern sub-regions of India	0-30 cm	Elbaalawy et al. (2016)

In recent years, machine learning techniques, particularly artificial neural networks (ANNs), have emerged as powerful alternatives to conventional statistical models for predicting soil properties and nutrient availability. Owing to their capacity for nonlinear mapping and self-adaptive learning, ANNs have demonstrated notable success in a range of soil science applications, including nutrient evaluation (Li et al., 2014), estimation of available nitrogen, phosphorous and K (Wu et al., 2014) without accounting for the interrelationships among multiple K pools. Moreover, many of these studies have not provided explicit predictive equations or interpretable coefficient outputs, thereby constraining their application in operational nutrient management and decision-support systems.

In response to these knowledge gaps, this study aimed to develop and validate a suite of ANN models capable of accurately estimating the distribution of multiple K fractions, including water-soluble, available (water-soluble + exchangeable), non-exchangeable, and total K prior to K amendment, and water-soluble, exchangeable, available, and fixed K following K amendment. Beyond model development, the trained ANN models were embedded into an open-source, Excel-based tool constructed within the Visual Basic for Application (VBA) framework, ensuring accessibility and practical usability of agronomists, soil scientists, and land managers. This integration bridges the gap between advanced computational modeling and field-level decision-making, thereby enabling data-driven, precision-oriented K management. The outcomes of this research are expected to contribute to a more comprehensive understanding of soil K dynamics, enhance fertilizer-use efficiency, and support the transition toward more sustainable and resilient agricultural systems.

The present study was guided by the following hypotheses: (1) ANNs can accurately predict multiple forms of soil K, using soil physicochemical properties and measured exchangeable K, (2) ANN-based approaches outperform traditional MLR models in predicting soil K fractions due to their superior ability to capture nonlinear interactions among soil parameters, and (3) the predictive performance of ANNs vary according to the chemical complexity of individual K fractions, with more complex fractions such as total K requiring deeper network architectures.

2. Materials and Methods

2.1. Dataset compilation

The two datasets utilized in this study were extracted from peer-reviewed articles published in international journals prior to 2019 (Table 1). Dataset 1 included soil properties (clay, sand, silt, OC, CEC, EC, and pH), water-soluble K, exchangeable K, available K (water-soluble + exchangeable), non-exchangeable K, and total K. Dataset 2 comprised the same soil properties, and initial water-soluble K, except that EC was not reported. In addition, dataset 2 contained dose-response data describing the relationships between KCl application rates (0–400 $mg.kg^{-1}$) and the resulting distribution of K among water-soluble, exchangeable, and fixed K forms.

Briefly, the authors listed in Table 1 determined particle size distribution using the hydrometer method and measured soil pH potentiometrically in a 1:2.5 soil: water suspension. The CEC measurement has been based on the ammonium acetate method at pH 7. Water-soluble K extracted with distilled water in a 1:5 (w/v) soil to water ratio, while exchangeable K extracted using 1 M ammonium acetate at pH 7. Non-exchangeable K quantified as the difference between K extracted by boiling nitric acid and the ammonium-acetate-extraction fraction, and total K determined following a complete digestion with a hydrofluoric acid mixture. Specifically, Portela et al. (2019) used a difference method to quantify fixed K, following the application of KCl at doses up to 400 $mg.kg^{-1}$. They derived fixed K using the following equation:

$$\text{Fixed K} = (\text{exchangeable K prior to K amendment} + \text{K amendment}) - \text{exchangeable K following K amendment} \quad [1]$$

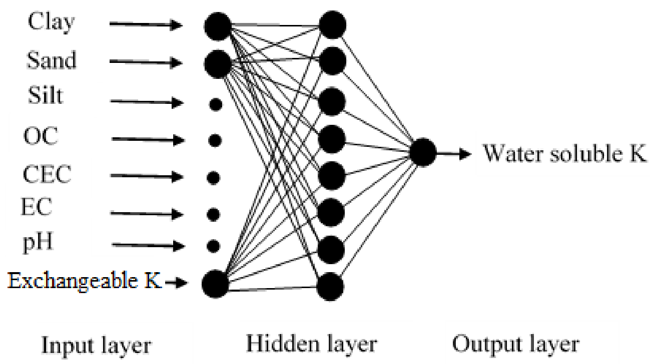


Fig. 1. A sample architecture of the artificial neural network model (ANN: 8-8-1) utilized to predict various fractions of soil K. As presented in Table 3, the ANNs implemented in this study vary in their input layer, number of hidden layers, number of nodes per hidden layer, and output layer.

Generally, the selection of articles, listed in Table 1 was carried out through a rigorous screening process, ensuring that only studies with comprehensive and consistent reporting of K fractions and soil properties were included. This approach enabled the compilation of a dataset that: (i) encompassed a broad spectrum of environmental and edaphic conditions, capturing substantial variations in elevation (relative to sea level), agro-ecological characteristics, climatic factors, soil horizons and depths, slope gradients, and parent materials; and (ii) maintained methodological consistency, thereby facilitating robust comparative analyses.

2.2. ANN models

During the second phase of the investigation, the two datasets were employed to construct multilayer perceptron ANN models using MATLAB software. The ANN-based modeling of individual K fractions was necessitated by disparities in data availability and experimental design between the two compiled datasets. Consequently, the predictor variables for predicting K fractions prior to K amendment comprised clay, sand, silt, OC, CEC, EC, pH, and measured exchangeable K. For predicting K fractions following K amendment, the predictor variables were clay, sand, silt, OC, CEC, pH, initial water-soluble K, and fertilizer-derived K. Separate ANNs were developed for each target variable (K fraction). For the pre-amendment condition, these target variables were water-soluble, available (sum of water-soluble and exchangeable), non-exchangeable, and total K. For the post-amendment condition, the target variables were fixed, water-soluble, exchangeable, and available K. Each K fraction was thus configured with a specific set of inputs and a single output corresponding to its target K fraction.

A representative ANN architecture was depicted in Fig. 1, showing distinct input layers for the soil variables and a single output layer for the predicted K fractions. A comprehensive summary of the input-output configurations for all developed models was provided in the flowchart in Fig. 2. The complete dataset was partitioned into training (70%), testing (15%), and validation (15%) subsets to evaluate the model robustness using unseen data.

To compare the predictive performances of ANN and MLR approaches, a separate MLR model was constructed for each target variable. The same set of predictors used as inputs for the ANNs (i.e., those represented in the input layer of Fig. 2) were used as independent variables in the MLRs, while the corresponding ANN output variables were designated as the dependent variables. The predictive efficacy of both ANN and MLR modeling approaches for the various K fractions was assessed using the correlation coefficient (r) between the predicted and observed K fractions, along with the mean absolute error (MAE) and root mean squared error (RMSE). Finally, the aforementioned ANNs were embedded into Excel-based tool using the Visual Basic for Applications (VBA) programming framework. The tool and VBA codes were presented as supplementary online material.

3. Results

The analysis of compiled data from published literature (Table 1) revealed a substantial heterogeneity in soil properties and K fractions, underscoring the diverse characteristics of the studied soils (Table 2). This diversity was immediately apparent in the soil texture, which spans the entire textural triangle, encompassing everything from coarse, sandy soils to heavy clays. Such a wide spectrum of textural classes inherently influence key soil processes like water retention. Furthermore, critical indicators of soil health and fertility—OC and CEC—also exhibited marked variability. This pronounced disparity suggests that the soil represented a wide range of management histories, climatic conditions and inherent fertility levels. Most critically for this study, the various K fractions demonstrated extensive variation. The wide ranges observed in water-soluble K, exchangeable K and total K (long-term reserve) highlight stark differences in both the

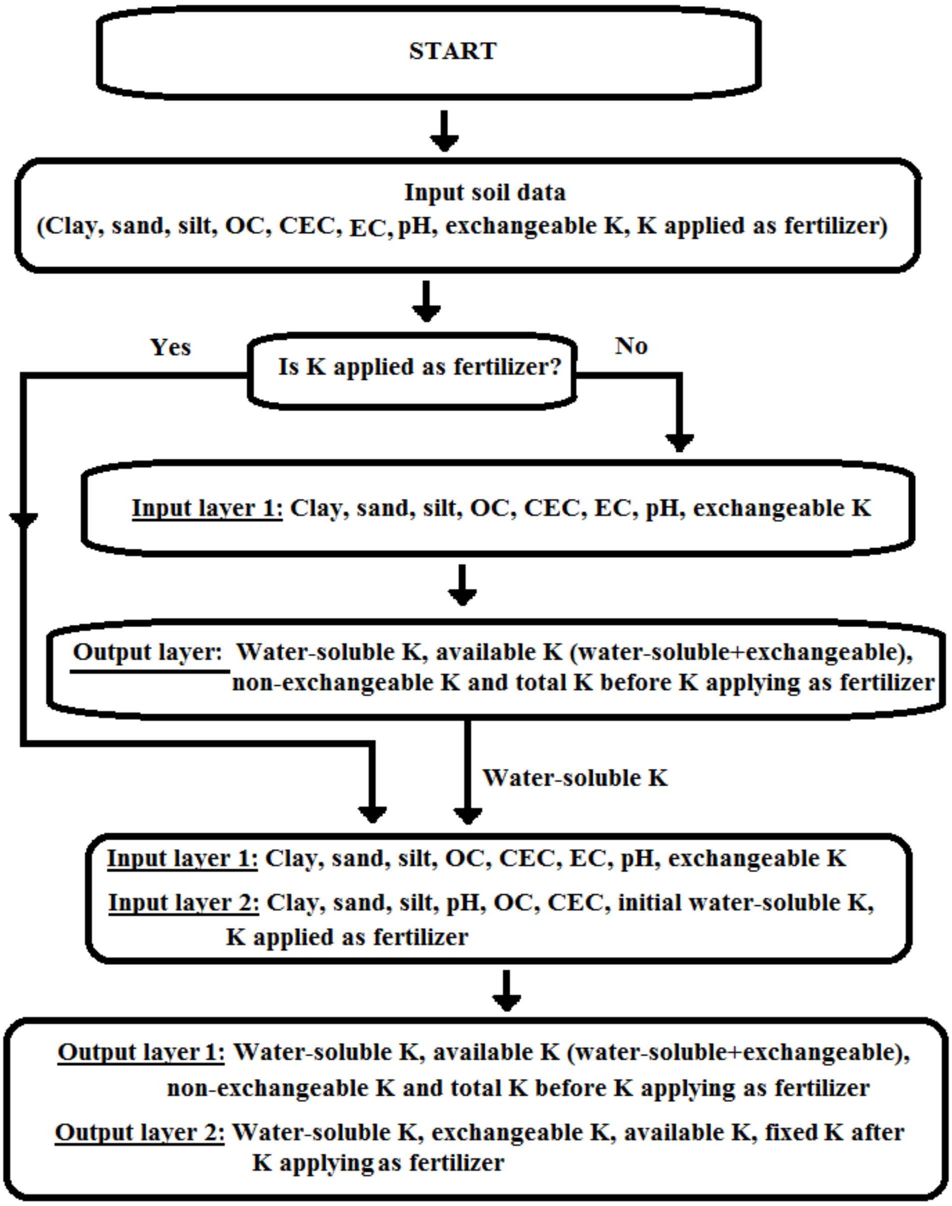


Fig. 2. Flowchart illustrating the prediction of various fractions of soil K using an Excel-based tool. The term "Added K" denotes the fertilizer-derived K input. Variation between the soil-property input layers (1 and 2) arises from constraints in the underlying datasets.

immediate K availability for plants and the total K reserves locked within soil matrix.

The ANN models demonstrated markedly superior predictive performance compared with the MLR models across all soil K fractions evaluated (Table 3). For water-soluble K prior to fertilization, the ANN model achieved a strong correlation between predicted and observed values ($r = 0.984$), markedly outperforming the MLR ($r = 0.780$). This model also produced sustainably lower errors (MAE = 8.73 vs. 47.61; RMSE = 23.83 vs. 84.43) and exhibited robust training, testing, and validation performance (0.992, 0.941, and 0.949, respectively). Similarly, the ANN for non-exchangeable K prediction achieved a high total-set correlation with markedly reduced error relative to MLR and strong split-sample performance [training (70%), test (15%), and validation (15%)]. The models for other K fractions followed the same pattern, with the ANN yielding substantially higher accuracy and far lower prediction errors, highlighting the ANN's advantage in modeling the complex interactions governing these fractions.

Following K amendment, ANN models again outperformed MLR across fixed, exchangeable, and water-soluble K fractions. Collectively, these results

Table 2. Summary of descriptive statistics for soil properties and K fractions used in the present study.

Attributes	Minimum	Maximum	Mean	Range
Clay (%)	3	68.7	35.85	65.7
Sand (%)	4	97	50.5	93
Silt (%)	0	60	30	60
OC (%)	0	5.97	2.99	5.97
CEC (cmol($^+$).kg^{-1})	0.6	62.56	31.58	61.96
EC (dS.m^{-1})	0.06	20.70	10.38	20.64
pH	5.27	8.77	7.02	3.50
Water-soluble K (mg.kg^{-1})	0	1332	666	1332
Exchangeable K (mg.kg^{-1})	5.083	1368.8	686.942	1363.72
Available K (water-soluble + exchangeable) K (mg.kg^{-1})	7	2700.8	1353.9	2693.8
Non-exchangeable K (mg.kg^{-1})	11.1	4200	2105.55	4188.9
Fixed K (mg.kg^{-1})	5	346	175.5	341
Total K (mg.kg^{-1})	674	21806.1	11240	21132.1

confirm that ANNs consistently captured the multivariate controls on soil K dynamics more effectively than MLR, producing higher correlations and substantially lower MAE and RMSE values across all K fractions.

The validation set performance consistently aligned with training and test results across all K fractions, demonstrating minimal overfitting. The close agreement among all three mentioned sets confirms that the models generalized effectively and are robust for predicting K dynamics beyond the data used for training.

4. Discussions

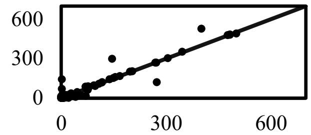
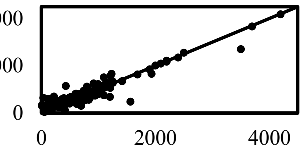
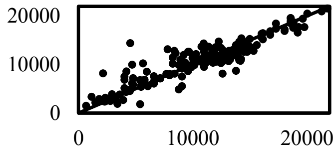
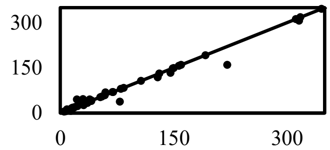
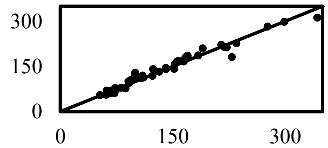
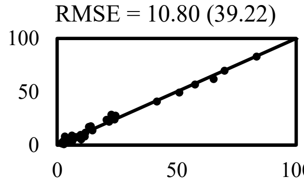
The substantial variability observed in the physicochemical properties and K fractions across the compiled dataset (Table 2) reveals the inherent heterogeneity of the studied soils and underscores the relevance of adopting ANN modeling approaches. The wide spectrum of textural classes fundamentally influences key soil processes such as water retention, aeration, and nutrient-holding capacity (Sparks, 1987). In particular, soils with higher clay content or greater proportion of 2:1 clay minerals (e.g. smectite, vermiculite) often exhibit greater capacity for K-fixation and buffering, whereas kaolinitic soils typically hold less inter-layer K and therefore lower total K reserves (Akbaş et al., 2017).

Similarly, the marked variability in soil OC and CEC across the dataset reflects a mixture of soils under differing management histories, climatic regimes, and parental material. High OC not only contributes to improved soil structure and moisture status but also influences nutrient metabolism and cation exchange processes, therefore affecting K availability (Six et al., 2002). As such, the wide disparity in OC and CEC signals soils with a broad range of fertility potentials and dynamic behavior (Weil and Brady, 2017).

Most critically for this study, the various K fractions exhibited extensive variation. The large ranges registered water-soluble K (the immediate available pool), exchangeable K (the short-term reserve) and total K (the long-term reserve/structural pool) highlight stark differences between soils in terms of both the immediate K supply to plants and the magnitude of K reserves locked in the mineral matrix (Sparks, 1987). These differences are further modulated by soil mineralogy: for instance, soils rich in feldspar or mica can possess significant non-exchangeable K that becomes available only slowly (Moterle et al., 2019).

In fact, the concept of a “K-paradox” has been discussed in the literature; although soils may contain large total K reserves, the plant–available portion may remain low or inaccessible due to fixation or slow release from non-exchangeable forms (Sparks, 1987; Weil and Brady, 2017). This variability and heterogeneity are particularly advantageous for the development and implementation of ANN models. Because the ANN training dataset spans a broad array of soil conditions, physicochemical property values and K fraction distributions, the resulting models are better equipped to capture the complex nonlinear, and multidimensional interactions inherent in soil-K systems. This enhances the generalization capacity and reliability of the ANN models when applied across diverse environmental and agricultural contexts. This superior performance is quantitatively confirmed, with the ANN models achieving correlation coefficients between 0.91 and 0.99, and lower prediction errors (MAE and RMSE) substantially outperforming the MLR models. This result is consistent with previous studies where ANNs outperformed linear or simpler statistical models in soil-related studies (Mosleh

Table 3. Performance evaluation of the multilayer perceptron (MLP) artificial neural networks (ANNs) and multiple linear regression models (MLRs) for predicting different soil K fractions, as qualified by the correlation coefficient (r), mean absolute error (MAE), and root mean squared error (RMSE). Values in parentheses denote MLR performance for comparative assessment.

@Network Identifier	Network architecture	*Training algorithm; sample size	correlation coefficient (r)			Axis titles of correlation charts	#Correlation plot with performance metrics for total set
			Training subset	Test subset	Validation subset		
Inputs: Soil traits, exchangeable K. Output: Water-soluble K prior to K amendment.	MLP 8-8-1	LM; 177	0.992	0.941	0.949	Predicted vs. observed soluble K (mg.kg^{-1})	 r = 0.984 (0.780); MAE = 8.73 (47.61); RMSE = 23.83 (84.43)
Inputs: Soil traits, exchangeable K. Output: Non-exchangeable K prior to K amendment.	MLP 8-8-8-1	LM; 177	0.973	0.891	0.909	Predicted vs. observed non-exchangeable K (mg.kg^{-1})	 r = 0.946 (0.725); MAE = 129.34 (311.39); RMSE = 197.24 (421.60)
Inputs: Soil traits, exchangeable K. Output: Total K prior to K amendment.	MLP 8-10-10-10-1	LM; 177	0.937	0.871	0.891	Predicted vs. observed total K (mg.kg^{-1})	 r = 0.916 (0.431); MAE = 1300.50 (3519.03); RMSE = 2037.11 (4341.22)
Inputs: Soil traits, initial water-soluble K, added K. Output: Fixed K following K amendment.	MLP 8-8-1	LM; 54	0.991	0.968	0.994	Predicted vs. observed fixed K (mg.kg^{-1})	 r = 0.987 (0.933); MAE = 11.04 (20.87); RMSE = 14.63 (31.44)
Inputs: Soil traits, initial water-soluble K, added K. Output: Exchangeable K following K amendment.	MLP 8-8-1	LM; 54	0.995	0.973	0.974	Predicted vs. observed exchangeable K (mg.kg^{-1})	 r = 0.991 (0.874); MAE = 8.13 (28.76); RMSE = 10.80 (39.22)
Inputs: Soil traits, initial water-soluble K, added K. Output: Water-soluble K following K amendment.	MLP 8-8-1	LM; 54	0.975	0.981	0.961	Predicted vs. observed soluble K (mg.kg^{-1})	 r = 0.990 (0.85); MAE = 1.97 (11.4); RMSE = 4.39 (16.68)

@: The input variables for the model differed as dictated by available data. For predicting K fractions following fertilizer K application, the input layer consisted of soil properties such as clay, silt, sand, pH, OC, and CEC. In contrast, models for all other K fractions prior to fertilization additionally included EC.

*: The Levenberg-Marquardt (LM) algorithm was employed as the optimization method in the training phase. The tangent sigmoid (TANSIG) and pure linear (PURELIN) transfer functions were used for the hidden and output layers, respectively.

#: In the charts, the solid line represents the 1:1 reference line.

et al., 2016; Mozaffari et al., 2024; Pacci et al., 2024; Tang et al., 2009).

The superior performance of ANNs over MLRs in this setting can be attributed to two key factors. First, the dynamic of K fractions are driven by a network of highly interrelated variables, i.e. the studied soil physicochemical properties, which result in nonlinear system behaviors, such as the accelerated release of K from non-exchangeable pools when exchangeable K falls below a specific level (Portela et al., 2019). Second, the ANN architectures were customized to capture this complexity. Easier-to-predict fractions were modeled with simpler structures (8-8-1), whereas the more complex non-exchangeable K required a moderately deep network (8-8-8-1), and total K, encompassing all pools, necessitated the most intricate design (8-10-10-10-1). This tiered complexity in network architecture reflects the gradation in soil processes, a principle observed in other nutrient modeling research (Li et al., 2014; Pacci et al., 2024).

From a mechanistic perspective, the high correlation between predicted and observed K fractions suggest that the models have implicitly captured key soil K dynamics. These dynamics include the exchange between solution and exchangeable pools, as well as the slow release of K from non-exchangeable interlayer sites in clay minerals and the weathering of K-bearing minerals such as mica and feldspar, processes often driven by soil acidification (Moterle et al., 2019). Furthermore, the models reflect the influence of soil texture and mineralogy, where a higher clay content enhances K buffering capacity. This reduces the rapid loss of exchangeable K but can also limit its immediate availability (Sparks, 1987). Finally, soil OC and CEC are represented as key modulating factors, influencing cation exchange equilibrium, K adsorption-desorption dynamics, and root access to K (Palanivell et al., 2020).

In terms of practical implications, the techniques developed here (ANN-embedded Excel + VBA tool) offer a readily accessible and user-friendly means for field practitioners, agronomists and soil-fertility managers to estimate multiple K fractions using routine soil analytics (clay, silt, sand, pH, CEC, EC, exchangeable K, fertilizer-derived K). This is valuable because conventional laboratory fractionation of K (water-soluble, exchangeable, non-exchangeable, and structural) is time-consuming, costly and not widely available in many regions. The user tool therefore provides a cost-effective alternative for site-specific K-management decisions. Moreover, by enabling prediction of both immediate K supply (water-soluble, exchangeable) and longer-term reserve K (non-exchangeable, structural), the tool supports a more holistic K-fertility strategy, enabling optimization of fertilizer scheduling, avoiding over-application (and potential environmental loss) and enhancing soil fertility (Xu et al., 2020).

Nevertheless, despite the strength of the present modeling approach, the future research directions should be noted. First, while the input dataset covers a wide range of soils, it may still omit certain soil types (e.g., highly calcareous soils, organic soils, extreme weathered Ferralsols) or cropping systems (e.g., biochar amendments, regenerative agriculture) that alter K dynamics in non-standard ways. Second, although the model inputs include routine soil properties, key factors such as clay mineralogy, specific surface area and weathering indices (alkali–Kaolinization index and chemical index of alteration) are not directly represented, even though these factors strongly influence non-exchangeable K (Zareian et al., 2018). Future models might integrate mineralogical or spectroscopic proxies (e.g., XRD-derived clay-mineral proportions of VIS-NIR spectra) to enhance predictive accuracy and mechanistic interpretability.

5. Conclusion

The results presented here demonstrate that ANNs provide a powerful and adaptable framework for predicting soil K fractions from readily measurable soil properties. By leveraging the intrinsic complexity and heterogeneity of soils, the developed models overcome many of the limitations of MLR, enable more accurate nutrient-management decision-making and have strong potential for extension to other nutrients (e.g., N, P, Mg) and broader soil quality indices. As agriculture moves into the era of digital-soil-fertility management and precision nutrient application, such tools will be increasingly central to balancing productivity, environmental stewardship and resource sustainability.

Supplementary Online Material

The Excel-based tool is available at: https://drive.shahroodut.ac.ir/index.php/s/fayE0zUH16TQe2M

The Visual Basic for Applications (VBA) codes (48 pages) for the Excel-based tool is available for download at:
https://drive.shahroodut.ac.ir/index.php/s/PDvgtXC47zasmdH

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