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# Prediction of soil potassium forms using physicochemical properties and exchangeable potassium: II. Influence of soil properties on potassium distribution

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## Abstract

A quantitative understanding of the factors regulating potassium (K) distribution in soils is essential for optimizing nutrient management in agricultural systems, as K availability directly influences crop productivity and soil health. To systematically evaluate the drivers of K dynamics, a suite of artificial neural networks, coupled with Deep Learning Important FeaTures (DeepLIFT) attribution analysis, was employed to quantitatively assess the relative influence of key soil properties, including clay, silt, and sand content, pH, organic carbon (OC), cation exchange capacity (CEC), and electrical conductivity (EC), on four distinct K pools: water-soluble K, non-exchangeable K, fixed K, and total K. Additionally, the study investigated the association of soil initial water-soluble K and fertilizer K application rate with the fixation of K fertilizer to elucidate the relationship between them. Key findings revealed divergent drivers across K fractions, highlighting the complexity of K dynamics in soils. CEC emerged as the dominant factor influencing water-soluble K variability (+22.43%), underscoring its role in regulating K mobility. Clay content exhibited contrasting effects, positively influencing non-exchangeable K (+13.42%), total K (+20.59%), and fixed K (+13.81%), while negatively impacting water-soluble K (-14.38%). EC was the primary determinant of non-exchangeable K (+34.27%), suggesting salinity's role in K retention. In contrast, pH showed a strong association with fixed K (+26.58%), reflecting its influence on interlayer trapping within 2:1 clay minerals. To bridge predictive modeling and practical applications, a genetic algorithm was integrated into an open-source, user-friendly Excel-based tool. This tool enables farmers and agronomists to optimize soil conditions for maximizing the sum of water-soluble and exchangeable K (plant-available K), thereby supporting precision nutrient management. By elucidating soil-specific K dynamics and providing actionable insights, this research advances sustainable K stewardship. The tool is accessible for download at: https://drive.shahroodut.ac.ir/index.php/s/fayE0zUH16TQe2M

**Keywords**: Potassium fractions, Soil physicochemical properties, Artificial neural network, Genetic algorithm optimization, DeepLIFT feature attribution.

## 1. Introduction

Potassium (K) ranks among the abundant elements in the Earth's crust; however, only a small fraction of total soil K is present in a plant-available form at any given time (Zörb et al., 2014; Sparks, 1987). This limited bioavailability arises from the partitioning of K into distinct operationally defined soil fractions including water-soluble, exchangeable, non-exchangeable, fixed, and total K. Each of these K fractions is characterized by unique dynamics in mobility, accessibility and responsiveness to agricultural management practices.

The distribution and transformation of soil K are primarily controlled by soil physicochemical attributes such as texture (clay, silt, sand), cation exchange capacity (CEC), pH, organic carbon (OC), and electrical conductivity (EC), along with the mineralogical composition of soils (Zhao et al., 2021; Sharpley, 1989). For instance, clay-rich soils, especially those containing 2:1 phyllosilicates like vermiculite and illite, are known to fix K in interlayer sites, contributing to the stability of non-exchangeable and fixed K forms (e.g., Florence et al., 2017). Conversely, sandy soils tend to exhibit poor K retention due to their low surface area and limited CEC, resulting in enhanced K leaching (Brady and Weil, 2017).

Soil pH also plays a dual role in K dynamics. Acidic conditions can enhance the release of $K^+$ from primary minerals like feldspars and micas while promoting fixation in certain clay minerals; alkaline environments, on the other hand, may suppress mineral weathering and stabilize K in non-labile forms (Liu et al., 2020; Simonsson et al., 2009). OC generally improves CEC and microbial activity, but can also bind K in organo-mineral complexes, complicating its immediate availability (Solly et al., 2020). EC introduces additional complexity by influencing K mobility through ionic strength, competition with other cations, and salinity-related transformations (Yan et al., 2023).

While the influence of individual soil properties on K dynamics has been broadly recognized, the magnitude and direction of their specific contributions across different K fractions remain inadequately quantified. It is not yet clear, for example, whether a high CEC consistently enhances all K pools, or whether it preferentially promotes certain forms while suppressing others. Similarly, the extent to which soil properties such as pH, or OC influence the plant-available (water-soluble + exchangeable) K under varying soil conditions requires further investigation.

To examine these relationships, a validated ensemble of artificial neural networks (ANNs) was used to systematically evaluate the relative influence of key soil parameters on the distribution of K fractions. The soil parameters analyzed were clay, silt, sand, pH, OC, CEC, and EC. The target K fractions consisted of water-soluble, non-exchangeable, fixed, and total K. Additionally, the association of soil initial water-soluble K and K fertilizer application rate with the fixation of K fertilizer was investigated. This approach provides new insights into the complex, often non-linear interactions governing the distribution of soil K fractions.

To enhance practical applicability, the ANNs were incorporated into an open-source decision-support tool developed in Microsoft Excel. The tool includes a genetic algorithm (GA)-based optimization module, allowing for the identification of optimal soil characteristics and strategies to maximize sum of water-soluble and exchangeable K (representing total available K), under specific soil conditions. Available K was selected as the key fraction due to its agronomic importance and bioavailability to plants. The primary goal of this integration was to translate data-driven insights from ANN predictions into actionable guidance for soil management. The novelty of this approach lies in combining interpretable deep-learning models (via DeepLIFT) with GA-based soil optimization in a user-friendly platform, enabling end users to both understand the drivers of K dynamics and implement optimized nutrient strategies without requiring advanced computational expertise.

## 2. Materials and Methods

### 2.1. Computation of the influence of soil parameters on K fractionation

This study employed a suite of pre-trained ANNs developed and validated by Gholipoor (2025) to quantify the impacts of key soil physicochemical properties (soil parameters) on K fractionation. The ANNs were trained and validated using an extensive dataset encompassing a wide range of soil variability. Due to the heterogeneous nature of the input variables, which differed significantly in both units and magnitudes, the dataset was preprocessed using Min-Max normalization. This transformation scaled all continuous predictor variables (soil parameters) and response variables (K fractions) to a common range of -1 to 1, thereby minimizing feature dominance and ensuring equitable contribution of each variable during model training and inference.

To interpret the ANNs and assess the influence of individual soil parameters on K fractions, the Deep Learning Important FeaTures (DeepLIFT) attribution was utilized (Shrikumar et al., 2017). DeepLIFT, which was implemented in MATLAB software, employs a backpropagation-based approach to assign relative scores to input features, thereby quantifying the marginal effects of soil properties on K fractions. A zero-reference baseline (i.e., all inputs set to the normalized baseline of 0) was used to compare activation differences, and feature scores were aggregated by summing the contribution of each input neuron across all hidden layers to obtain the final relative influence of each soil property on a given K fraction. Aggregated scores were then normalized to 100% to enable direct comparison between predictor contributions. This approach facilitated a detailed decomposition of the ANN model predictions, providing mechanistic insights into the role of each soil parameter in governing K fraction concentrations.

Two separate DeepLIFT analyses were performed:

1) The first analysis assessed the relative contributions of clay, silt, sand, OC, CEC, EC, pH, and exchangeable K to the predicted levels of water-soluble K, non-exchangeable, and total K.
2) The second analysis examined the relative contribution of clay, silt, sand, OC, CEC, pH, water-soluble K, and fertilizer-derived K to the predicted levels of fixed K.

Where fixed K is calculated as follows (Portela et al., 2019):

Fixed K = (exchangeable K prior to K amendment + K amendment) – exchangeable K following K amendment

These two analyses were conducted separately because the sets of soil-property input layers differed due to constraints in the available datasets. For additional details, refer to Gholipoor (2025). Collectively, these analyses elucidated the nonlinear relationships between soil properties and K fractionation, identifying the dominant physicochemical drivers of K distributions in soil complexes.

### 2.2. Genetic Algorithm-based optimization of soil physicochemical properties for enhanced available (sum of water-soluble and exchangeable) K

To facilitate the translation of ANN model-derived insights into practical agronomic applications, a computational tool was developed within Microsoft Excel, utilizing Visual Basic for Applications (VBA) as the programming framework. As shown in Fig. 1, the tool integrates a GA optimization module, where pre-trained ANN models function as surrogate evaluators of solution fitness. The GA module was initialized with a population of 20 individuals (npop = 20; Fig. 1), each representing a candidate solution defined by soil parameters and K input from fertilizers. Optimization was set to run over a

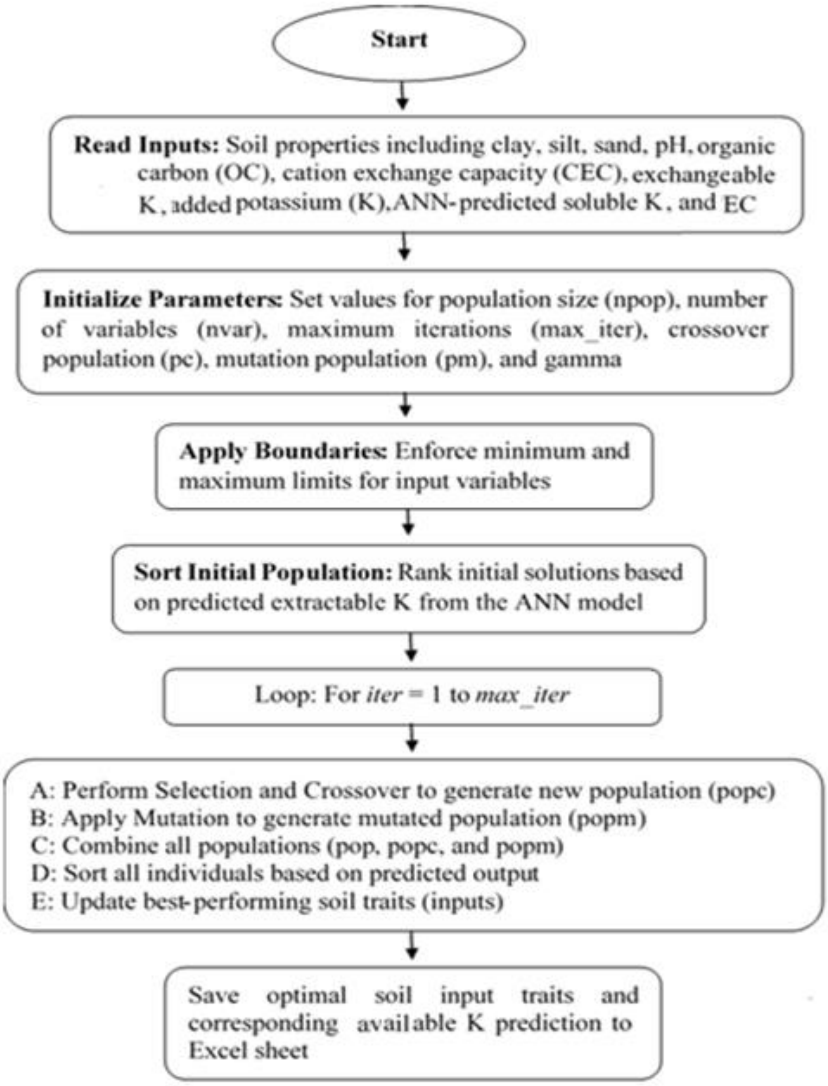


**Fig. 1.** Flowchart illustrating the use of a genetic algorithm (GA) within an Excel-based tool to predict available (exchangeable + water-soluble) K by optimizing key soil input parameters including pH, OC, CEC, added K (fertilizer-derived K), clay, silt, and sand.

maximum of 100 generations to enable convergence toward optimal or near-optimal solutions.

Crossover was performed using a blend-based strategy, where a gamma parameter ($\gamma = 0.1$) modulated the degree of offspring variation within the prescribed variable bounds, ensuring an optimal balance between exploration and exploitation in the GA. Parent selection was conducted via the roulette wheel method, incorporating a selection pressure coefficient ($\beta = 1$) to favor individuals with superior fitness. The crossover population size (popc) was set to 80% of the total population (npop), corresponding to a crossover probability (pc) of 0.8 (Fig. 1). Mutation was applied to 30% of npop (pm = 0.3; Fig. 1) to maintain population diversity and prevent premature convergence.

All variables were constrained within agronomically relevant bounds to ensure the feasibility of resulting solutions. The fitness of each individual was evaluated using a cost function tailored to soil-specific characteristics, including texture and soil initial water-soluble K. Through iterative refinement, the GA effectively identifiesd optimal combinations of soil physicochemical parameters that maximize sum of water-soluble and exchangeable K (representing total available K).

## 3. Results

The results indicated that CEC was the most influential predictor of the water-soluble K, explaining +22.43% of the variation, followed by soil pH (+16.04%) (Fig. 2). In contrast, soil exchangeable K content explained only +7.95% of the water-soluble K variation, suggesting that broader soil chemical properties play a more dominant role in water-soluble K variations. Notably, EC, clay, and

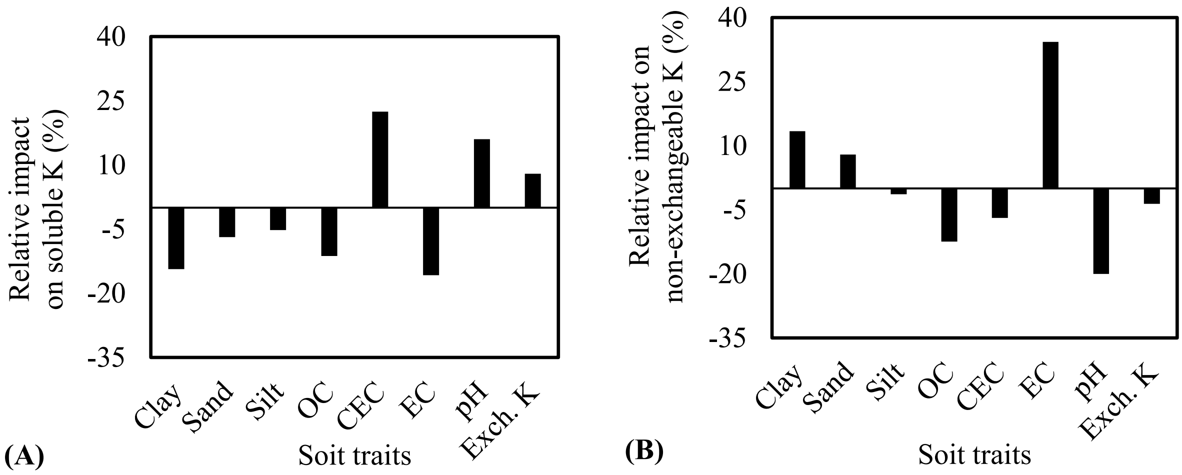


**Fig. 2.** Relative impact of soil properties including clay, sand, silt, organic carbon (OC), cation exchange capacity (CEC), electrical conductivity (EC), pH, and exchangeable K (Exch. K) on water-soluble K (A) and non-exchangeable K (B).

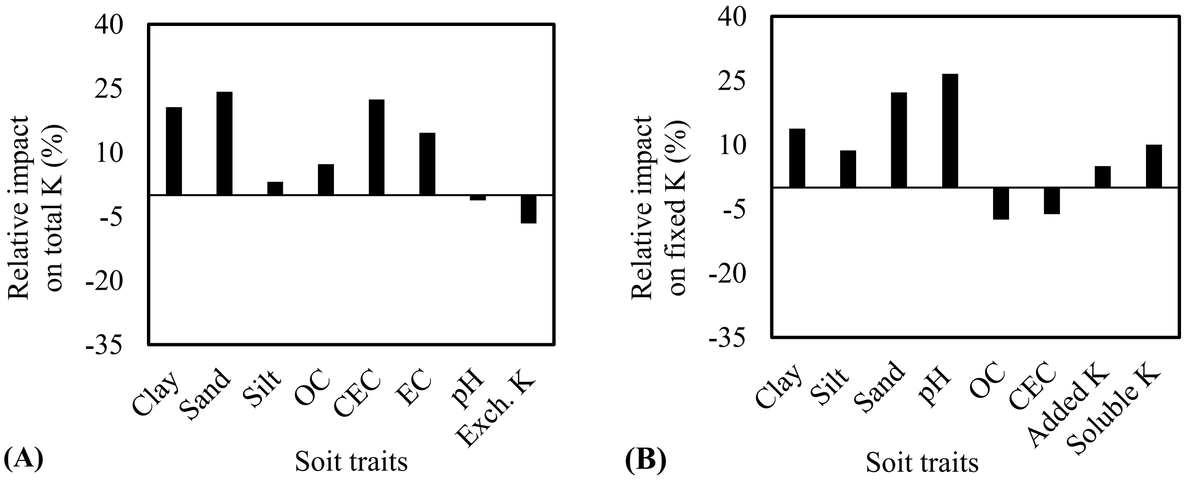


**Fig. 3.** (A) Relative impact of soil properties including clay, sand, silt, organic carbon (OC), cation exchange capacity (CEC), electrical conductivity (EC), pH, and exchangeable K (Exch. K) on total soil K. (B) Relative impact of soil properties (clay, silt, sand, pH, OC, CEC), fertilizer-derived K (added-K), and initial water-soluble K on proportion of fixed K following fertilization. Variation in horizontal axes of panels (A) and (B) occurs because the two analyses were based on separate datasets. For more detail, refer to Gholipoor (2025).

OC exhibited negative contributions, indicating potential inhibitory or interactive effects.

EC was identified as the primary positive predictor of non-exchangeable K, accounting for +34.27% of the observed variation (Fig. 2). Clay and sand also showed a considerable positive influence. In contrast, pH and OC had a decreasing effect (-20.03% and -12.45%, respectively), suggesting a secondary role in non-exchangeable K variations. CEC demonstrated a marginal negative association (-6.91%) with this fraction of K, possibly due to competitive interactions.

Among the predictors, sand and CEC showed the strongest positive influences on total K, with impacts of approximately +24.21% and +22.38%, respectively, followed by clay (+20.59%) (Fig. 3). These results suggest that soil properties enhancing cation retention, such as clay minerals and high CEC, play a key role in accumulation of total K, while the positive effect of sand may reflect the presence of K-rich primary minerals in sandy fraction. Silt and pH exert minimal effects, indicating limited influence on total K. Notably, exchangeable K displays a weak association, which may not imply a true reduction in total K but rather a statistical artifact in the model used to estimate relative contributions.

As shown in Fig. 3, pH exerted the strongest positive influence on K fixation following K fertilization, with relative impact of approximately +26.58%. Sand content followed closely with a +22.23% effect, while clay content showed a +13.81% relative impact, suggesting that soils with higher pH or greater proportions of sand and clay tend to immobilize more K following K amendment. OC and CEC had a marginal decreasing effect, implying that soils rich in OC or possessing high CEC are less prone to fix K. At higher rates of K amendments (added K) and elevated levels of initial water-soluble K, a greater proportion of applied K tends to become fixed in the soil. This is evidenced by the positive impacts shown in Fig. 3.

# 4. Discussion

## 4.1. Clay

This study utilized an ensemble of ANN models, interpreted through DeepLIFT feature attribution, to quantify the relative influence of soil physicochemical properties on various K fractions. The results revealed a distinct hierarchy in the influence of soil clay content on the distribution of different K fractions. As expected, clay content positively influenced non-exchangeable K (+13.42%), consistent with the established understanding that clay-rich soils contain larger reserves of structurally bound and interlayer K. Numerous studies support this relationship; for example, Sharpley (1989) reported high coefficients of determination ($R^2$ = 0.66–0.90) between clay content and mineral K across diverse soil types, while Güzel et al. (2001) demonstrated that non-exchangeable K is predominantly associated with the clay minerals, particularly smectitic.

In contrast, the DeepLIFT analysis indicated a negative attribution of clay content to water-soluble K (-14.38%). This finding does not contradict the general principle that clayey soils possess greater total K. Rather, it reflects the relative influence of clay content on variation in the immediately available pool. Because the soluble, exchangeable and non-exchangeable pools are tightly integrated and buffered, high clay content often enhances K retention on exchange sites and promotes interlayer fixation. These processes can reduce the proportion of K present in the water soluble fraction, even when absolute K quantities are high. This interpretation is further supported by the positive influence of clay on fixed K (+13.81%), consistent with the role of fine-textured soils in incorporating K into mineral lattices (Bilias and Barbayiannis, 2019).

## 4.2. Silt

Silt content appeared to exert a nuanced influence on K dynamics. Specifically, it exhibited a modest negative effect on water-soluble K (-5.25%), while positively contributing to non-exchangeable (+7.92%), fixed (+8.66%), and total soil K (+3.16%). The positive association between silt and fixed K aligns with the concept of silt-rich soils acting as a buffering reservoir for plant-available K (Zörb et al., 2014). The relatively large specific surface area of silt particles enhances its capacity to retain K ions through weak electrostatic forces and physical entrapment within micro-aggregates. Enhanced soil aggregation and moisture retention in silt-dominated matrices may further facilitate K accessibility to plant roots by maintaining a hydrated diffusion pathway (Brady and Weil, 2017). Moreover, silt derived from granitic or felsic parent materials can serve as a significant source of K through weathering of K-bearing minerals such as feldspars and micas, contributing to the long-term K supply in agroecosystems.

## 4.3. Sand

Sand content negatively influenced water-soluble K (-6.89%), consistent with its low CEC and high leaching potential (Havlin et al., 2014). In contrast, sand contributed positively to less labile K fractions, including non-exchangeable (+7.92%), fixed (+22.23%), and total K (+24.21%). These pools are primarily associated with K-bearing minerals such as feldspars and micas, which are concentrated in the sand and silt fractions. Sadusky et al. (1987) reported that up to 88.70% of total K in sandy soils from Atlantic Coastal Plain resided in the sand fraction, predominantly within K-feldspars. Notably, fine sand particles exhibited greater K release than coarser ones, highlighting the influence of particle size on K availability. While sand-dominated soils may contain substantial total K reserves, their agronomic utility is limited unless weathering or biological processes facilitate mobilization (Zörb et al., 2014).

## 4.4. pH

Soil pH significantly influenced K distribution, exhibiting a positive effect on water-soluble (+16.04%) and fixed K (+26.58%). This suggests that alkaline conditions may enhance K desorption from labile sources while promoting fixation within 2:1 clay interlayers (e.g., vermiculite, illite), particularly during drying-rewetting cycles that facilitate interlayer expansion (Sparks, 1987). Conversely, pH negatively affected non-exchangeable (-20.03%), and total K (-1.20%). Although elevated pH can improve short-term K availability by reducing $H^+$ competition at exchange sites (Havlin et al., 2014), it may also facilitate long-term fixation and reduce mineral weathering. The dissolution of K-bearing silicates (e.g., orthoclase, micas) is typically proton-driven; thus, weathering rates may decline under alkaline conditions. However, certain micas may undergo hydroxyl-driven weathering at high pH (Köhler et al., 2003), indicating mineral-specific responses.

## 4.5. OC

OC exerted a negative effect on water-soluble K (-11.28%). This suppression is likely due to the formation of stable organo-mineral complexes, particularly with clay and silt particles, which can sequester K ions and reduce their concentration in the soil solution. Within these complexes, $K^+$ mobility is restricted through a combination of electrostatic attraction within the diffuse double layer of organic coatings and physical encapsulation within soil aggregates (Hinsinger et al., 2005). It is important to contextualize this interaction because complexes formed between monovalent $K^+$ and organic ligands are inherently less stable than the strong, specific bonds formed by divalent cations (e.g., $Ca^{2+}$, $Mg^{2+}$) and far less stable than the very strong fixation of $K^+$ within the interlayer sites of 2:1 phyllosilicate clays (Römheld and Kirkby, 2010).

Furthermore, OC demonstrated consistent negative effects on both non-exchangeable (-12.45%) and fixed K pools (-7.51%). This pattern reinforces the premise that OC has a limited direct interaction with specific mineral phases responsible for intermediate to long-term K retention. The presence of abundant OC may indirectly compete for adsorption sites on the edges of clay minerals or disrupt the diffusion of $K^+$ into interlayer positions, thereby favoring its maintenance in more readily available, exchangeable forms rather than in fixed or non-exchangeable forms (Sparks, 1987). Consequently, while enhancing soil OC is broadly beneficial for soil health, its role in K dynamics is complex; it appears to promote K distribution skewed away from both the immediately soluble and strongly fixed pools, potentially increasing the dominance of the exchangeable fraction in the overall K equilibrium.

### 4.6. CEC

CEC was positively associated with water-soluble (+22.43%) and total K (+22.39%), reaffirming its critical role in K retention within the soil solution and broader K reservoirs (Sparks, 1987). However, in apparent contrast to some classical views, the present DeepLIFT analysis revealed that CEC exerted marginal negative effects on the non-exchangeable and fixed K (-6.19%) pools. This distinct distribution pattern suggests that in high-CEC soil, K is preferentially maintained in the water-soluble and total pools, while its transition into less labile, fixed forms is comparatively limited.

The mechanisms underlying this distribution are twofold. First, the high-CEC environment is characterized by intense competitive adsorption, where divalent cations such as $Ca^{2+}$ and $Mg^{2+}$ often outcompete monovalent $K^+$ for occupancy on the general exchange complex. This competition can limit the specific portion of exchange sites occupied by K, thereby constraining the pool of readily exchangeable K despite high total reserves. Second, while the overall fixation is minor, high-CEC phyllosilicates like smectites possess dynamic interlayers that can temporarily entrap $K^+$ ions (Gurav et al., 2024). This reversible fixation acts as a short-term sink, further modulating the immediate availability of exchangeable K.

From an agronomic perspective, these dynamics may create a risk of K depletion in high-CEC soils. Despite their capacity to hold large total K reserves, cation competition and reversible K entrapment may restrict its immediate availability in the exchangeable pool. Under intensive cropping, replenishment of this pool may not meet plant demand, leading to a paradox where high total K coincides with crop deficiency. Therefore, management should not rely on total K alone. Instead, regular monitoring of exchangeable K and split fertilizer applications are essential to prevent transient deficiency and leverage the soil's innate retention capacity for sustainable production.

The positive relationship between CEC and clay content notwithstanding, as they govern distinct K pathways. Clay primarily mediates mineralogical fixation (i.e., interlayer and lattice incorporation), which sequesters K from the soil solution. CEC, conversely, quantifies the capacity to retain K in an exchangeable, and thus plant-available, form (Sparks, 1987). This mechanistic distinction is reflected in present DeepLIFT attribution analysis, which assigns opposing conditional effects to these two predictors when modeled concurrently. Specifically, the positive attribution of clay content to non-exchangeable K (+13.42%) surpassed the negative attribution of CEC (-6.91%) to this K fraction, demonstrating that entrapment mechanism dominated it within the system. A parallel trend was observed for fixed K following fertilizer K amendment (Fig. 3).

Furthermore, the results regarding OC and CEC appear contradictory because OC often contributes to CEC. However, the model results reflect conditional and mechanistically distinct influences: OC can raise CEC while simultaneously reducing water-soluble K through formation of organo-mineral complexes, physical encapsulation within aggregates, and restricted diffusion (Marschner, 2012). Conversely, the positive effect of CEC on water-soluble K likely reflects the portion of CEC derived from mineral surfaces (particularly high-activity clays), which tends to retention of K in the exchangeable/solution phase (Mengel and Kirkby, 2001). Importantly, when both variables increase together, as often occurs in soils with concurrent organic enrichment and high clay reactivity, their opposing effects on water-soluble K do not cancel out fully. Instead, the stronger positive influence of CEC (+22.43) outweighs the negative influence of OC (-11.28%), resulting in net positive tendency toward greater water-soluble K. Thus, OC and CEC operate through distinct, opposing mechanisms on solution K, and the DeepLIFT attributions correctly capture these conditional, co-occurring effects, which together explain the apparent contradiction.

### 4.7. EC

The dynamics of K showed a shift in its speciation from readily available forms to more stable, fixed pools as salinity (EC) increased. In contrast to the decline in water-soluble K (-15.78%), EC exhibited a strong positive association with non-exchangeable K (+34.27%), indicating that K is not lost but rather distributed into less accessible forms. This pattern is fully consistent with the mechanisms expected under high ionic strength: (i) abundant soluble cations such as $Na^+$ displace $K^+$ from the soil solution and exchange sites, and (ii) the displaced $K^+$ becomes increasingly fixed within clay interlayers (Sparks, 1987). Under saline-alkaline conditions, elevated pH further reinforces this trend by promoting K fixation and suppressing its bioavailability (Rengasamy, 2010; Zörb et al., 2014). Therefore, despite the moderate positive effect of EC on total K (+14.58%), this accumulation does not translate into plant-available K. Instead, physicochemical constraints imposed by salinity and alkalinity dominate K speciation. Therefore there is no contradiction between high total K and low available K: salinity drives K into non-exchangeable pools, reducing nutrient-use efficiency even when overall K reserves appear sufficient.

### 4.8. Association of soil initial water-soluble K and fertilizer application rate with the fixation of K fertilizer

As provided in Fig. 3, both initial water-soluble K and fertilizer-derived (added) K promote K fixation, with approximately +5.00% and +10.00% effects, respectively, indicating that greater K availability increases the conversion of exchangeable K into non-available forms. The smaller effect of initial water-soluble K is due to its steady background concentration, which gradually enhances diffusion of K into interlayer sites of 2:1 clays (Sparks, 1987). In contrast, the larger effect from fertilizer-derived K likely results from temporary high concentration of fertilizer K in soil solution immediately after application, creating a strong driving gradient favoring rapid interlayer entrapment (Marschner, 2012; Mengel and Kirkby, 2001). It has been evidenced that pulses of K fertilizer can be readily fixed, whereas equivalent increments of soluble native K are fixed more slowly (Havlin et al., 2014). Consequently, repeated K additions can progressively increase non-exchangeable K pools, affecting long-term K availability (Zörb et al., 2014). These results highlight that fertilizer K has a greater tendency (+10.00%) to be fixed than native water-soluble K (+5.00%), emphasizing the need for optimized timing and rate of application to minimize fixation-related K losses.

## Summary and Conclusion

The results revealed distinct controlling factors for each K pool:

- Water-soluble K was primarily influenced by CEC, contributing +22.43% to its variability.
- Non-exchangeable K was most strongly determined by EC (+34.27%), indicating the role of ionic strength in $K^+$ fixation, particularly in saline-alkaline soils.
- Fixed K exhibited a strong relationship with soil pH (+26.58%), likely due to its effect on K entrapment within the interlayers of 2:1 clay minerals.

*Key implications include:*

- Tailored K fertilization strategies are essential in saline soils to mitigate K fixation under high EC conditions.
- Soils with elevated OC may require additional K supplementation to compensate for potential temporary immobilization.
- Consideration of clay mineralogy and soil pH is critical for long-term K management, balancing availability with retention.

Further research should focus on expanding the model's capabilities across a much broader range of agroecosystems and incorporating more K fractions in the ANN models.

**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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