JJEES

JJEES (2026) 17 (3): 287-292
ISSN 1995-6681

Jordan Journal of Earth and Environmental Sciences

Ionic Strength Prediction Using Selected Physicochemical Properties of Calcareous Soils: A Case Study from Al-Hashimya Area, Zarqa Governorate, Jordan

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Received on 24 September 2025; Accepted on 26 January 2026

Abstract

Accurate estimation of ionic strength (I) is essential for predicting soil solution chemistry and ion interactions in calcareous soils, where carbonate equilibria dominate. Direct measurement of ionic strength requires full ionic analysis, which is costly and time-consuming; therefore, developing reliable, locally calibrated predictive relationships with easily measured soil properties is of practical value. This study aimed to establish empirical models linking ionic strength with electrical conductivity (EC) and sodium adsorption ratio (SAR) in calcareous soils from the Al-Hashimya area, Zarqa Governorate, Jordan. Forty-three surface soil samples (0–15 cm) from urban areas were analyzed for pH, EC, major cations and anions, and $CaCO_3$ content. Ionic strength was computed from measured ion concentrations and compared with EC-based models using linear and multiple regression. Results revealed that EC ranged from 1.3 to 63.8 dS m^{-1} and I from 0.025 to 0.94 mol L^{-1}, with a strong linear correlation ($R^2 = 0.91$) between EC and I. The best-fit model for these calcareous soils was $I = 0.0304 + 0.0155\ EC_{25}$, which yielded an R^2 22% higher than the widely used Griffin and Jurinak (1973) equation, reflecting the higher charge density and ion pairing characteristic of carbonate-rich systems. Incorporating SAR and key ionic species (Na^+, Cl^-, Ca^{2+}, Mg^{2+}, and HCO_3^-) further improved model performance ($R^2 > 0.95$). The locally calibrated model provides a practical tool for soil salinity assessment and irrigation management in the Al-Hashimya region, while highlighting the broader need for composition-aware ionic-strength calibrations across diverse calcareous soil systems.

Keywords: *soil salinity, ionic strength, calcareous soils, SAR, $CaCO_3$, Al-Hashimya, Zarqa*

1. Introduction

Calcareous soils are those soils containing abundant free $CaCO_3$ and often a calcic horizon. They are widespread across the world's drylands and are thought to make up more than one-third of the earth's land surface, according to FAO (2016). In the World Reference Base (WRB), such soils commonly fall within Calcisols, which are defined (among other criteria) by secondary carbonate enrichment and a calcium carbonate equivalent ≥ 15% over ≥ 15 cm of the profile. The amount of $CaCO_3$ in these soils can range from hardly detectable to 95% (Marschner, 1995). The prevalence of calcareous materials in arid and semi-arid regions reflects restricted leaching and frequent pedogenic carbonate accumulation, leading to alkaline pH, Ca–Mg–HCO_3-dominated solutions, and distinctive nutrient and physical behavior. The high accumulation of carbonates influences soil characteristics linked to plant growth, such as soil water relations and the availability of plant nutrients, as discussed extensively by Marschner (1995) and the contemporary soil chemistry literature.

Ionic strength (I) is the most critical attribute governing electrostatic interactions in soil solutions, and activity coefficients translate concentrations into thermodynamic activities. Accurate activities support predictions of mineral solubility, metal speciation, surface complexation/adsorption, and ion-exchange equilibria that regulate nutrient availability and contaminant mobility in calcareous settings.

Directly computing I from full-ion analysis is labor- and cost-intensive, particularly when routine monitoring or spatial mapping is required. By contrast, electrical conductivity (EC) is quick to measure, widely standardized (at 25 °C), and directly connected to salinity assessment in soil science and irrigation practice (e.g., ECe from saturated paste extracts and in situ ECa surveys). This has motivated long-standing efforts to infer comprehensive solution chemistry—including total dissolved solids, major-ion loads, and ionic strength—from EC. An influential contribution is the work of Griffin & Jurinak (1973), which linked ionic strength linearly to EC in natural waters and soil extracts. Variants of this relation (e.g., $I \approx 0.0127 \times EC_{25}$, with I in mol L^{-1} and EC in dS m^{-1} at 25 °C) remain embedded in practice and guidance. However, such calibrations are empirical and therefore sensitive to solution composition and temperature, with the original datasets dominated by monovalent Na–Cl systems, and do not account for the distinctive carbonate-rich composition of calcareous soil solutions.

Soil physicochemical characteristics chemistry, such as EC, SAR, and ionic strength, which are significant factors

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influencing soil chemical characteristics, including clay dispersion and flocculation (Emerson, 1977; Goldberg & Forster, 1990; Miller et al., 1990). The osmotic stress between clay particles decreases as the electrolyte concentration rises, until it reaches a point where short-range van der Waals forces take control and lead to flocculation.

Despite the widespread occurrence of calcareous soils across drylands and their carbonate-dominated chemistry, composition-aware calibrations that translate routine measurements (e.g., EC, SAR, pH) into reliable estimates of ionic strength remain scarce in the peer-reviewed soil literature.

This study has three specific objectives:

1. To establish empirical, calibration-based relationships linking ionic strength (I) with electrical conductivity (EC) in calcareous soils of the Al-Hashimya area, Zarqa Governorate, Jordan;
2. To evaluate whether incorporating sodium adsorption ratio (SAR) and key ion species (Na^+, Cl^-, Ca^{2+}, Mg^{2+}, HCO_3^-) improves predictive accuracy beyond EC-alone models;
3. To provide a practical, composition-aware tool for rapid ionic strength estimation to support irrigation management and soil salinity assessment in the region.

2. Materials and Methods

2.1 Study area and sampling

Forty-three (n = 43) urban surface soils (0–15 cm) were collected across the Al-Hashimya area in the Zarqa Governorate, Jordan. The study was limited to urban surface areas to maximize accessibility and representativeness within a constrained geographic scope. Sites were purposively selected to span a wide range of pH, $CaCO_3$ content, and salinity to ensure adequate representation of the diversity of soil solution chemistry typical of the region. At each site, several scoops within ~10 m were composited, placed in labeled, airtight bags, and kept shaded during transport. In the lab, samples were air-dried at room temperature, gently disaggregated by hand, and passed through a 2-mm sieve. Subsamples for alkalinity and ion analysis were sealed in airtight containers to limit CO_2 exchange until extraction, following established soil salinity protocols (Rhoades, 1996; Corwin & Yemoto, 2017).

2.2 Saturated paste extract and analytical procedures

Saturated soil pastes were prepared and extracted under vacuum following USDA standard methodology (Richards, 1954). pH and electrical conductivity (EC) were measured immediately after extraction at ambient laboratory temperature and subsequently normalized to 25 °C using the standard temperature correction function. EC values are reported at 25 °C (EC_{25}). Filtered extracts were analyzed for Na^+, K^+, Ca^{2+}, Mg^{2+}, Cl^-, HCO_3^-, and SO_4^{2-}. Cations were measured by Atomic Absorption Spectrophotometry (AAS). Chloride and sulfate were determined by ion chromatography following standard EPA (1993) methods.

All electrical conductivity measurements throughout this manuscript refer exclusively to the electrical conductivity of saturated paste extracts normalized to 25 °C (EC_{25}). This standardization is essential because the validity of EC-I relationships depends critically on the extraction method and temperature normalization.

2.3 Soil and solution parameters

The values obtained from ion analysis were used to calculate two key descriptors:

Sodium Adsorption Ratio (SAR) following Richards (1954) and Ayers & Westcot (1985):

$$SAR = [Na^+] / \sqrt{(([Ca^{2+}] + [Mg^{2+}]) / 2)} \quad (1)$$

where cation concentrations are in mmolc L^{-1}.

Ionic Strength (I):

$$I = \tfrac{1}{2} \Sigma\, c_i\, z_i^2 \quad (2)$$

where z_i and c_i are the charge and molar concentration of the ionic species (Sposito, 2016), measured in mol L^{-1}.

2.4 Carbonate system speciation and activity coefficient calculations

The measurement of CO_3^{2-} directly in soil solution is analytically challenging due to its rapid equilibration with atmospheric CO_2 and its instability during storage and transport. Therefore, CO_3^{2-} concentrations were calculated from measured pH and HCO_3^- using the Henderson-Hasselbalch equation and carbonate equilibrium constants for the bicarbonate buffer system at 25 °C:

$$pH = pKa2 + \log([CO_3^{2-}]/[HCO_3^-]) \quad (3)$$

where, pKa2 = 10.33 (at ionic strength ≈ 0.1 mol L^{-1} and 25 °C; Sposito, 2016).

CO_3^{2-} was calculated as:

$$[CO_3^{2-}] = [HCO_3^-] \times 10\text{^}(pH - pKa2) \quad (4)$$

Assumptions underlying this approach:

1. Soil solutions are assumed to be in equilibrium with respect to the carbonate buffer system (Richards, 1954).
2. A fixed pCO_2 is not imposed; rather, the Henderson-Hasselbalch equation relies on the measured pH and HCO_3^- concentration, implicitly accounting for the solution's CO_2 buffering capacity (Sposito, 2016).
3. Deviation from equilibrium due to CO_2 loss during sampling was minimized by sealing subsamples in airtight containers until extraction and analysis, following established protocols (Rhoades, 1996).

Activity coefficients for all ionic species were calculated using the Davies equation (Davies, 1962) with ionic strength computed from Equation (2), following standard practice in soil chemistry (Sposito, 2016).

2.5 Modeling the $EC_{25} \rightarrow I$ relationship

To translate routine EC measurements into ionic strength, we evaluated:

- M_0: $I = 0.0127 \times EC_{25}$ (Griffin & Jurinak, 1973) as a historical baseline;

- M_1: $I = \beta_0 + \beta_1 EC_{25}$ (linear model, EC-only);
- M_2: $I = \beta_0 + \beta_1 EC_{25} + \beta_2 SAR$ (linear model with SAR);
- M_3: Multiple regression incorporating ion species and $CaCO_3$ content.

Models were fit by ordinary least squares (OLS) with robust standard errors; performance was summarized with R^2, root mean square error (RMSE), mean absolute error (MAE), and bias.

3. Results and Discussion

3.1 Soil salinity, sodicity, and basic chemistry

The electrical conductivity of the soil paste extract (EC_{25}) spanned nearly two orders of magnitude (1.3–63.8 dS m^{-1}), while pH ranged from slightly acidic to moderately alkaline (6.7–8.5). Sodium dominated the soluble cations (up to ~35 meq L^{-1}), followed by Ca^{2+}, whereas Cl^- exceeded SO_4^{2-} among the anions. Summary statistics (minimum, maximum, and coefficient of variation, CV) are reported in Table 1. The high coefficients of variation in EC_{25} (98.71%) and SAR (113.03%) indicate marked spatial heterogeneity typical of calcareous, irrigated arid soils where localized irrigation patterns, soil parent material variation, and differential salt accumulation create complex salinity distributions.

Table 1. Descriptive statistics of key soil-solution properties

Property	Min	Max	CV (%)
Ph	6.71	8.50	5.27
EC_p (dS m^{-1})	1.30	63.80	98.71
SAR	0.75	51.85	113.03
Ionic strength, *I* (mol L^{-1})	2.5×10^{-2}	0.94	91.72
Total anions	2.2×10^{-2}	0.66	94.11
Total cations	9.0×10^{-3}	0.75	119.10
Ion activity product, IAP = $a(Ca^{2+})\cdot a(CO_3^{2-})$	2.0×10^{-5}	3.1×10^{-3}	110.53
$CaCO_3$ (%)	26.64	62.41	23.74

3.2 Saturation state with respect to calcite

At 25 °C, the thermodynamic solubility product for calcite is:

$$Ksp = [Ca^{2+}] \times [CO_3^{2-}] = 10^{-8.42} \quad (5)$$

The saturation index (SI) indicates the stability of a mineral in a particular solution:

$$SI = \log_{10}(IAP/Ksp) \quad (6)$$

where IAP is the ion activity product. SI > 0 indicates supersaturation and a tendency toward calcite precipitation, whereas SI < 0 indicates undersaturation and potential dissolution.

The measured IAP range (2.0×10^{-5} to 3.1×10^{-3}) far exceeds Ksp, implying SI ≫ 0 and supersaturation with respect to calcite—consistent with carbonate-rich soils where high pH and low pCO_2 elevate CO_3^{2-} activities. Supersaturation indicates a tendency for secondary $CaCO_3$ precipitation and pedogenic carbonate accumulation. This finding explains the high $CaCO_3$ content (26.64–62.41%) observed in these soils and demonstrates the importance of understanding carbonate equilibria for predicting soil chemical processes, including the formation and stabilization of secondary carbonate horizons typical of calcareous soils in arid regions.

3.3 Linking ionic strength to EC and solution composition

Because ionic strength (I) governs activity coefficients via electrostatic screening, many practical models relate I to the easily measured EC. For natural waters and soil extracts dominated by monovalent ions (e.g., Na^+–Cl^- systems), the classic Griffin & Jurinak relationship is $I = 0.0127 \times EC_{25}$. This model was established using datasets that do not adequately represent carbonate-dominated systems with high divalent-cation content.

In the calcareous soils of this study, the best linear fit between measured I and EC_{25} was:

$$I\ (mol\ L^{-1}) = 0.0304 + 0.0155\ EC_{25}\ (dS\ m^{-1}),\ R^2 = 0.910 \quad (7)$$

Table 2. Linear relationships between ionic strength and EC from literature and this study

Relation	Reference	The relation between actual and predicted
I=0.016×EC I in mol/L and EC in dS/m	Ponnamperuma et al., (1966)	y = 3.5108x - 0.0243 R^2 = 0.9098
I= 0.0127×EC I in mol/L and EC in dS/m	Griffin and Jurinak (1973)	y = 0.7607x - 0.0053 R^2 = 0.9098
Is = 0.0446EC-0.000173 I in mol/L and EC in mS cm^{-1}	Gillman and Bell (1978)	y = 2.6097x - 0.0182 R^2 = 0.9098
I = 0.0304+0.0155*EC_{25} I in mol/L and EC in dS/m	Present study	y = 0.907x + 0.0241 R^2 = 0.9098

The slope of Eq. (7) is slightly higher than that of Griffin–Jurinak, reflecting the higher average charge density (greater divalent Ca^{2+} and Mg^{2+} content) and ion pairing in carbonate systems. Formation of ion pairs such as $CaHCO_3^+$ reduces the number of free ions in solution relative to total dissolved solids, affecting the EC-I relationship. This mechanistic insight explains why composition-aware models are necessary for accurate ionic strength prediction in systems with significant carbonate buffering.

3.4 Ionic composition and correlations

Model M_1 achieves 22.3% higher R^2 compared to the historical M_0 (Griffin & Jurinak, 1973) model, reducing RMSE by 51.6% (from 0.128 to 0.062 mol L^{-1}). The addition of SAR in M_2 provides marginal further improvement (ΔR^2 = 0.016; 2% increase), reducing RMSE from 0.062 to 0.054 mol L^{-1}. For rapid field or routine laboratory predictions when SAR measurements may not be readily available, the simpler M_1 (EC-only) model offers substantial practical improvements over existing methods. However, when SAR and ion speciation data are available, model M_2 offers the highest predictive accuracy.

Table 3. Performance metrics for different models

Model	Description	R^2	RMSE (mol L^{-1})	MAE (mol L^{-1})	Bias (mol L^{-1})
M_0	$I = 0.0127 \times EC_{25}$ (Griffin & Jurinak, 1973)	0.744	0.128	0.095	-0.032
M_1	$I = 0.0304 + 0.0155\ EC_{25}$ (locally calibrated linear)	0.910	0.062	0.048	+0.008
M_2	$I = 0.0298 + 0.0149\ EC_{25} + 0.0031$ SAR Linear with SAR	0.926	0.054	0.041	+0.003
M_3	$I = f(EC_{25}, SAR, Cl^-, HCO_3^-, Na^+, Ca^{2+}, Mg^{2+}, \%CaCO_3)$	0.958	0.018	0.012	+0.001

3.5 Ionic composition and correlations

Pearson correlations (Table 4) underline EC_{25}'s strong association with key soluble ions. The exceptionally high EC-Cl^- correlation (r = 0.98) indicates that chloride is the dominant anion controlling solution salinity in these soils, typical of salinized arid-region soils where irrigation with marginally saline water concentrates chloride. The strong EC-Na^+ correlation (r = 0.93) reflects co-mobilization of sodium with chloride (sodic-saline type salinity pattern). In contrast, EC shows moderate correlations with Ca^{2+} (r = 0.65) and Mg^{2+} (r = 0.78), indicating that divalent cations contribute substantially to ionic strength via their charge-squared weighting in Equation (2), even though their molar concentrations are lower than Na^+.

CEC and organic matter (OM%) show weak associations with EC_{25} in this dataset, consistent with salinity being driven primarily by the dissolved ion pool rather than by exchange capacity at the sampled spatial scale (urban surface soils with variable land use and irrigation history).

Table 4. Pearson correlations for selected soil parameters and ions

	pH	EC_{25}	Cl^-	HCO_3^-	Na^+	Ca^{2+}	Mg^{2+}	I calculated
pH	1.00							
EC_{25}	-0.46	1.00						
Cl^-	-0.48	0.98	1.00					
HCO3-	-0.013	0.29	0.27	1.00				
Na	-0.46	0.93	0.94	0.15	1.00			
Ca	-0.49	0.65	0.63	0.09	0.75	1.00		
Mg	-0.32	0.78	0.77	0.58	0.70	0.53	1.00	
I calculated	-0.47	0.95	0.95	0.41	0.94	0.76	0.87	1.00

The correlation of I with EC_{25} (r = 0.95) validates the strong predictive relationship captured by Equation (7) and justifies the use of easily measured EC as a surrogate for ionic strength in this calcareous-soil context.

3.6 Multiple regression incorporating ion species and carbonate content

Incorporating composition further improves prediction; multiple regression analysis identified Cl^-, HCO_3^-, Na^+, Ca^{2+}, Mg^{2+}, and $CaCO_3$% as significant covariates. The resulting model is:

$$I = -2.4\times10^{-2} + 1.7\times10^{-3}\ EC_{25} + 4.3\times10^{-4}[Cl^-] + 2.1\times10^{-3}[HCO_3^-] + 5.0\times10^{-4}[Na^+] + 9.1\times10^{-4}[Ca^{2+}] + 1.1\times10^{-3}[Mg^{2+}] + 5.6\times10^{-4}\ \%CaCO_3 \quad (8)$$

where,

- I: ionic strength (mol L^{-1})

- EC_{25}: electrical conductivity at 25 °C (dS m^{-1})

- $[Cl^-]$, $[HCO_3^-]$, $[Na^+]$, $[Ca^{2+}]$, $[Mg^{2+}]$: ion concentrations (mol L^{-1})

- $\%CaCO_3$: calcium carbonate content (percent by mass)

Note on Equation (8) application: All ion concentrations must be expressed in mol L^{-1}. Concentrations measured in other units (mmol L^{-1}, meq L^{-1}, mg L^{-1}) must be converted to mol L^{-1} using appropriate molecular weights before substitution into the equation.

This model achieves $R^2 > 0.95$, providing high predictive accuracy. The dominance of Cl^- and HCO_3^- coefficients reflects the importance of the primary dissolved salt composition in determining ionic strength through charge-concentration relationships. While pH, K^+, CEC, and OM were tested in the multiple regression, they were removed during model selection, indicating they do not significantly improve the prediction once major ion concentrations are accounted for.

3.7 Application of the derived I–EC model in spatial prediction

The locally calibrated ionic strength model was applied to interpolated EC values across the study area using ordinary kriging spatial prediction. EC values were interpolated to a regular grid using sample-based kriging with an exponential semivariogram model. Subsequently, the derived I-EC relationship [Eq. (7)] was applied to all interpolated EC grid values to generate spatially explicit predictions of ionic strength distribution.

The spatial analysis reveals distinct zones of high ionic strength (I > 0.6 mol L^{-1}) concentrated in the northeastern quadrant of the study area, corresponding to regions with the highest EC values. Moderate-salinity zones (0.3 < I < 0.6 mol L^{-1}) form a transition band, while low-salinity areas (I < 0.3 mol L^{-1}) occur predominantly in western and southern

portions of the study area. This spatial heterogeneity reflects local variations in irrigation practices, soil parent material composition, and hydrogeological factors driving salt accumulation.

The spatial distribution of ionic strength directly informs targeted salinity management strategies. High ionic strength zones require the following practices:

1. Enhanced irrigation scheduling and salt leaching
2. Selection of salt-tolerant crop varieties
3. Potentially, separate water management protocols

Low-salinity zones may support a wider range of crops with minimal salinity constraints. This practical application demonstrates the utility of the locally calibrated I-EC model for region-specific irrigation planning and soil amendment strategies.

3.8 Study limitations and generalizability

This study has several important limitations that should be acknowledged:

1. Geographic scope: Sampling was limited to the urban Al-Hashimya area, Zarqa Governorate, Jordan. Results represent only surface soils (0–15 cm) from this localized region and cannot be directly generalized to calcareous soils in other geographic areas or different soil depths without independent validation.
2. Soil type specificity: The derived models are calibrated for the distinctive ionic composition of these particular soils (dominated by Na^+-Cl^- salinity with significant carbonate buffering). Different calcareous soil systems with alternative dominant salt compositions (e.g., Ca^{2+}- SO_4^{2-} systems) may require separate calibrations.
3. Model validation: The models presented are based on a single dataset (n = 43 samples) from one time period. External validation using independent samples from the same region, as well as comparison with other calcareous-soil regions, is recommended before widespread practical application.
4. Practical application scope: While Eq. (7) (M_1: simple EC-only model) provides substantial improvement over the Griffin & Jurinak (1973) universal equation, its use should be limited to the Al-Hashimya region where it was calibrated. Application to other regions should be preceded by local model development using the methodology described here.

Despite these limitations, this study provides:

- A methodological framework for developing composition-aware I-EC calibrations in carbonate-dominated systems
- Quantitative evidence that local calibrations substantially improve ionic strength prediction
- A practical tool specifically applicable to irrigation management in the Zarqa region

4. Conclusions

For calcareous soils in the Al-Hashimya area (Zarqa Governorate, Jordan), the locally calibrated model provides superior predictive accuracy compared to the widely applied Griffin & Jurinak (1973) equation, yielding a 22% improvement in explanatory power and reducing prediction error (RMSE) by 52%. This substantial improvement reflects the higher divalent-cation content and carbonate-induced ion pairing characteristic of these Zarqa region soils.

Incorporation of key ion species (Cl^-, HCO_3^-, Na^+, Ca^{2+}, Mg^{2+}) and $CaCO_3$ content further refined predictions to $R^2 > 0.95$, providing maximum predictive accuracy when complete ion analysis is available. For routine field applications where only EC and SAR are measured, adding SAR to the simple EC model (M_2) yields a marginal improvement ($\Delta R^2 = 0.016$) and may not always justify the additional measurement effort, depending on available laboratory resources.

The practical application of this locally calibrated model to irrigation management in arid regions is demonstrated through the spatial prediction of ionic strength distribution across the study area. The methodology presented here provides a template for developing similar composition-aware I-EC calibrations in other calcareous-soil regions, emphasizing that reliable ionic-strength prediction requires region-specific calibration rather than relying on universal equations that do not account for local compositional patterns.

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