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Integrating GIS, principal component analysis and Python for groundwater quality assessment in the Khemisset–Tiflet aquifer, Morocco

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ABSTRACT

Groundwater quality assessment is essential for sustainable water resource management in semi-arid regions, where increasing anthropogenic pressures and natural hydrogeochemical processes significantly influence groundwater composition. The Khemisset–Tiflet aquifer, located in northwestern Morocco, constitutes a major source of water for domestic and agricultural uses but remains vulnerable to quality degradation. This study aims to characterize the physicochemical properties of groundwater and investigate the dominant factors controlling its hydrochemical variability through an integrated and reproducible analytical framework. A total of 34 groundwater samples were collected during the May 2018 field campaign. In situ measurements included pH, temperature, electrical conductivity (EC), total dissolved solids (TDS), salinity, dissolved oxygen, and depth to groundwater level. Complementary laboratory analyses of selected major and trace elements were performed for seven highly mineralized sampling stations using ICP-AES. Spatial variability was investigated using Geographic Information Systems (GIS), while multivariate statistical analysis was performed through principal component analysis (PCA) implemented in Python using open-source scientific libraries. The results revealed pronounced spatial heterogeneity in groundwater mineralization, with highly mineralized groundwater occurring in specific sectors of the aquifer. Electrical conductivity ranged from 2 to 8408 µS cm^{-1}, while TDS varied between 1 and 5633 mg L^{-1}. PCA highlighted strong associations among EC, TDS, and salinity, reflecting their common mineralization signal, while a secondary dimension was mainly associated with temperature and depth to groundwater level. The observed spatial patterns are consistent with the combined influence of groundwater circulation and water–rock interaction, although the relative contribution of natural and anthropogenic processes cannot be established from the available dataset. The integrated use of field measurements, GIS, and Python-based multivariate analysis provides a transparent framework for characterizing groundwater-quality variability and establishes a baseline for future monitoring of the Khemisset–Tiflet aquifer.

Keywords: groundwater quality, physico-chemical parameters, principal component analysis, Python, GIS, Khemisset–Tiflet, Morocco.

INTRODUCTION

Groundwater constitutes one of the most valuable freshwater resources worldwide and plays a fundamental role in sustaining domestic water supply, agricultural production, and industrial development, particularly in semi-arid and arid regions where surface water resources are limited.

In Morocco, groundwater represents a strategic resource that supports socio-economic development and food security. However, increasing water demand, recurrent droughts associated with climate change, rapid agricultural intensification, and urban expansion have considerably increased pressure on groundwater resources, leading not only to quantitative depletion but also to progressive deterioration of groundwater quality.

The scarcity of surface water resources and their temporal irregularity encourages local populations to exploit groundwater resources, often without adequate knowledge of the geometry of the underlying aquifers or of their potential. The Khemisset-Tiflet region, part of the Sebou hydraulic basin, has experienced considerable agricultural development in recent years, and water demand has increased significantly with the expansion of irrigated areas. Despite this growing pressure, few hydrogeological or hydrochemical studies have been conducted in this specific sector, the most directly relevant prior work being a localized assessment of anthropogenic impacts on shallow groundwater quality in the Tiflet city area (Qoutbane et al., 2020), which did not address the broader Khemisset-Tiflet aquifer investigated here. A more appropriate qualitative and quantitative understanding of aquifer characteristics and behavior is therefore needed to support more sustainable groundwater exploitation and sound water-resource management in this region.

Groundwater quality is controlled by complex interactions between natural hydrogeological processes and anthropogenic activities. Natural mechanisms such as mineral dissolution, water–rock interaction, ion exchange, and residence time govern the hydrochemical evolution of groundwater, whereas agricultural practices, fertilizer application, wastewater infiltration, and excessive groundwater abstraction may significantly alter its chemical composition. These combined processes generate strong spatial variability in groundwater quality, making its characterization particularly challenging in heterogeneous aquifer systems.

During the last decade, multivariate statistical techniques have become essential tools for interpreting complex hydrochemical datasets. Among these techniques, principal component analysis (PCA) has proven particularly effective for reducing data dimensionality, identifying correlations among physicochemical variables, and distinguishing the dominant processes controlling groundwater chemistry. Simultaneously, Geographic Information Systems (GIS) have become indispensable for visualizing spatial variations and identifying groundwater quality patterns that support water-resource management.

Recent advances in open-source scientific computing have further transformed environmental data analysis. Python has emerged as one of the most widely adopted programming languages in hydrogeology because of its transparency and extensive scientific ecosystem. Libraries such as pandas, NumPy, scikit-learn and Matplotlib enable efficient preprocessing, statistical analysis, and visualization. In the present study, this computational framework was used as a working tool to process and interpret the hydrochemical dataset; it is presented as part of the applied methodology rather than as a methodological novelty in itself, since the combination of hydrochemical analysis, GIS and PCA is by now a well-established approach in groundwater studies, as illustrated by several recent applications across Morocco and other semi-arid regions (Taoufiq et al., 2023; Benyoussef et al., 2024; Bouib et al., 2024; El-Rawy et al., 2024; Gautam et al., 2024; Kaibi et al., 2025).

Although numerous studies have investigated groundwater quality in Morocco using conventional hydrochemical analyses and multivariate statistical methods, the Khemisset–Tiflet aquifer specifically has received comparatively little attention, This regional knowledge gap, rather than the analytical tools themselves, constitutes the principal motivation and contribution of the present study.

The present study addresses this gap by combining field measurements, laboratory analyses, geographic information systems, and principal component analysis to characterize groundwater quality in the Khemisset–Tiflet aquifer. Specifically, the objectives are to (i) characterize the physicochemical properties of groundwater collected from 34 sampling sites, (ii) evaluate the spatial variability of groundwater quality using GIS-based mapping, (iii) identify the principal hydrochemical factors controlling groundwater composition through principal component analysis, and (iv) provide a baseline hydrochemical characterization of this specific, previously undocumented aquifer that can support future groundwater monitoring and management.

MATERIALS AND METHODS

Study area

The study was conducted in the Khemisset–Tiflet aquifer, located in northwestern Morocco within the Sebou River Basin. The study area extends over approximately 1600 km^2 and lies between the cities of Rabat and Meknes, covering the Khemisset and Tiflet regions. The aquifer constitutes an important groundwater resource supporting domestic water supply, irrigation, and other socio-economic activities in this semi-arid region.

From a geological perspective, the study area is situated at the transition between the western Meseta and the southern Rif domain. This geological setting results in a heterogeneous hydrogeological environment characterized by variable lithological formations and complex groundwater circulation. Groundwater recharge mainly occurs through rainfall infiltration and surface-water interactions, whereas groundwater discharge is controlled by pumping, natural drainage, and regional hydraulic gradients.

The region experiences a Mediterranean semi-arid climate characterized by irregular rainfall, high evapotranspiration rates, and increasing pressure on groundwater resources due to agricultural development and population growth. These environmental conditions make groundwater quality monitoring essential for sustainable water-resource management. The location of the study area is presented in Figure 1.

Groundwater sampling and physicochemical analysis

A preparatory phase preceded the field campaign, consisting of an exhaustive inventory and careful review of existing water points across the study area. This inventory enabled the selection of a final network of 34 representative water points, which was structured into a georeferenced database under ArcGIS 9.3, ensuring spatial coverage of the main hydrogeological units and groundwater exploitation zones prior to the field measurements described below.

A groundwater sampling campaign was conducted during the normal hydrological season in May 2018 to assess the physicochemical characteristics of groundwater in the Khemisset–Tiflet aquifer. A total of 34 groundwater samples were

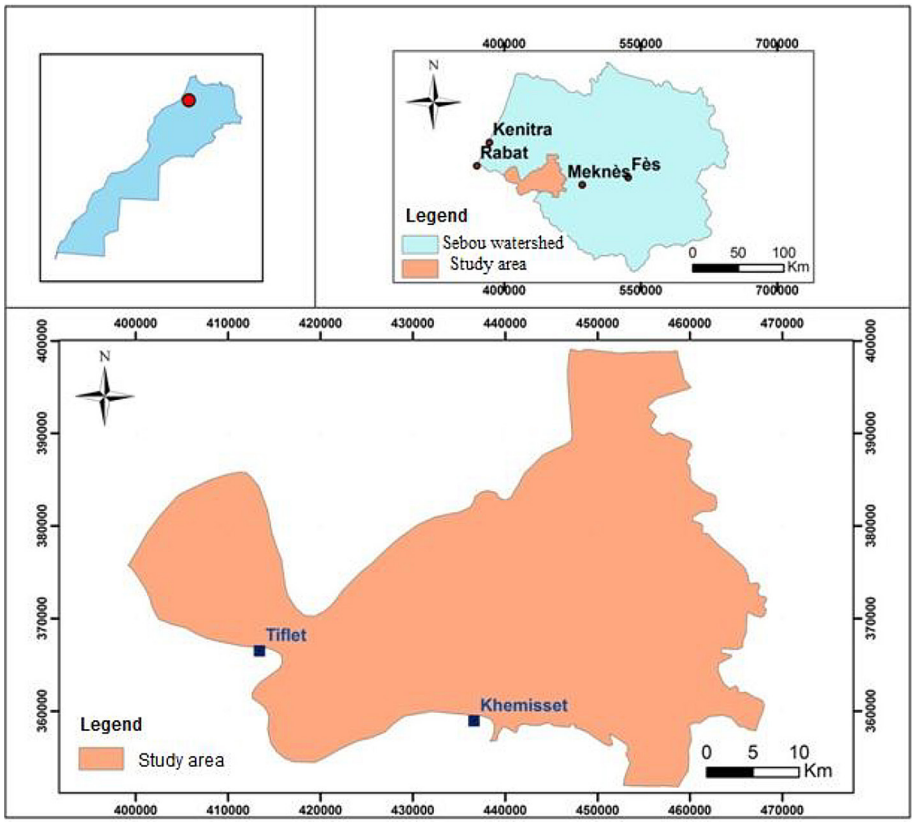

Figure 1. Location of the study area within the Sebou watershed, Morocco

collected from wells distributed throughout the study area to ensure representative spatial coverage of the main hydrogeological units and groundwater exploitation zones. At each sampling location, the geographic coordinates, well depth, piezometric level, lithological characteristics, soil type, and groundwater exploitation mode were recorded.

Field measurements were performed immediately after groundwater abstraction using a KLL-Q2 multiparameter piezometric probe, allowing simultaneous measurement of piezometric level and in situ physicochemical parameters. The measured parameters included pH, water temperature, EC, TDS, salinity, and DO, which provide essential information on groundwater mineralization and hydrochemical conditions. Electrical conductivity, salinity, and TDS values were read directly from the probe display in the field.

These seven stations were selected among the sites exhibiting the highest electrical conductivity, salinity, and TDS values, in order to characterize the chemical composition of the most mineralized groundwater in the aquifer. Consequently, this subset does not constitute a spatially representative sample of the aquifer as a whole, and the corresponding major/trace-element results (Section 3.8) should be interpreted as indicative of the most mineralized sector only, rather than generalized to the entire study area. Samples designated for major/trace-element analysis were kept cool and protected from light, preferably at 4 °C, until transport to the laboratory of the Cité de l'Innovation, Sidi Mohamed Ben Abdellah University (USMBA), Fez, where the concentrations of calcium (Ca), sodium (Na), magnesium (Mg), aluminum (Al), chromium (Cr), iron (Fe), manganese (Mn), and phosphorus (P) were determined by Inductively coupled plasma atomic emission spectroscopy (ICP-AES) using an internal analytical method developed at the laboratory of Cité de l'Innovation. Detailed instrumentation settings, calibration standards, and detection limits for these analyses are not available.

The spatial distribution of the sampling points across the study area is presented in Figure 2.

Statistical analysis

The hydrochemical dataset was subjected to descriptive and multivariate statistical analyses to investigate the relationships among the measured physicochemical parameters and to identify the dominant factors controlling groundwater quality. Prior to analysis, the dataset was checked for consistency and completeness. Because the measured variables were expressed in different units and exhibited different ranges of variation, they were standardized (z-score normalization) to ensure equal weighting in the multivariate analysis; no assumption of multivariate normality was applied as a criterion for PCA. Pearson's correlation analysis was first performed to evaluate the linear relationships between the physicochemical parameters. PCA was then applied to the standardized

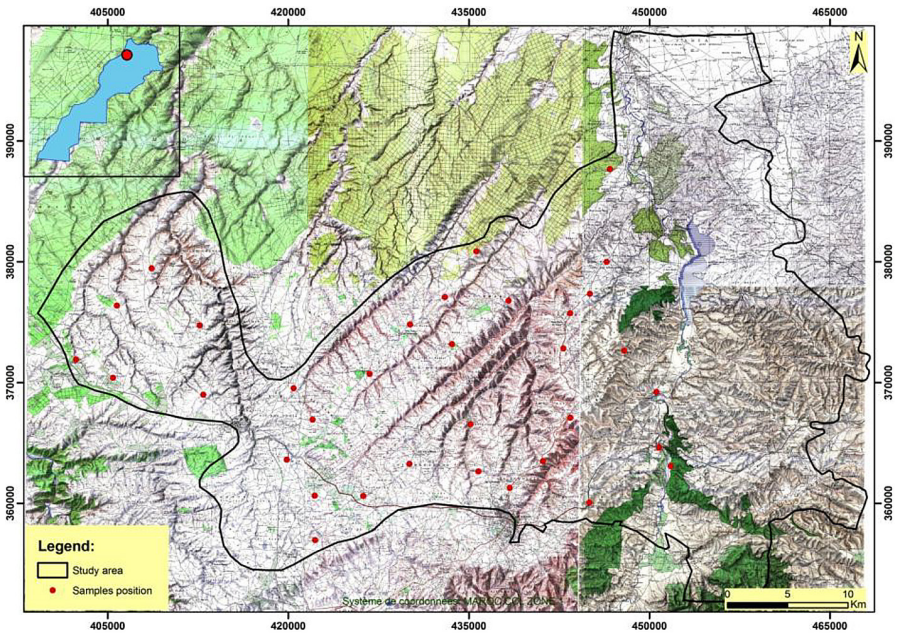

Figure 2. Location of the groundwater sampling points

correlation matrix to reduce data dimensionality while preserving the maximum amount of information contained in the original dataset. Each sampling site was treated as an observation (row) and each physicochemical parameter as a variable (column), following the classical PCA framework introduced by Pearson (1901) and later formalized by Hotelling (1933) (Cahuzac and Bontemps, 2008). The principal components were ranked according to their eigenvalues, and the first two components — accounting for the largest share of total variance — were retained for graphical interpretation using loading and score plots.

Nine active variables were included in the PCA: NP (depth to the groundwater level below ground surface, measured at the well head, m), T (groundwater temperature, °C), Cond (electrical conductivity, µS/cm), Sal (salinity, g/L), TDS (total dissolved solids, mg/L), H2O (water density, g/L, as recorded by the multiparameter probe), pH, O2 (dissolved oxygen concentration, mg/L), and %O2 (dissolved oxygen saturation, %). Sampling station identifiers (S1–S34) were used only as observation labels and were not entered as active variables in the analysis.

Computational framework

Data processing and statistical analyses were performed in Python (version 3.13.15; Python Software Foundation, 2026) within the Google Colab computing environment. The following libraries were used: pandas (version 2.2.3), for tabular database management and preprocessing; scikit-learn (version 1.6.1), for the standardization procedure and Principal Component Analysis, chosen for its flexibility, reproducibility, and integration with advanced statistical validation tools; and Matplotlib (version 3.10.0) and Seaborn (version 0.13.2), for initial graphical analyses and visualization of the correlation and factorial-map results. The workflow consisted of five successive steps: (i) data organization and preprocessing, (ii) data standardization, (iii) Pearson correlation analysis, (iv) Principal Component Analysis, and (v) graphical visualization and interpretation of the results.

GIS-based spatial analysis

GIS were employed to analyze the spatial distribution of groundwater quality and groundwater flow within the Khemisset–Tiflet aquifer. The geographic coordinates of the sampling locations, together with the physicochemical and piezometric data collected during the field campaign, were integrated into a GIS database.

Spatial interpolation of groundwater quality parameters and piezometric levels was performed using the Ordinary Kriging method under ArcGIS 9.3, based on a spherical semi-variogram model, following an approach comparable to recent applications combining semivariogram-based kriging with multivariate water-quality analysis (Masood et al., 2022). Kriging is a geostatistical interpolation technique that estimates values at unsampled locations by considering the spatial autocorrelation among neighboring observations.

Spatial distribution maps were generated for EC, and piezometric level. These maps were used to identify spatial trends in groundwater mineralization and to support the interpretation of groundwater flow patterns across the study area.

RESULTS

Table 1 summarizes the descriptive statistics (minimum, maximum, mean, and standard

Table 1. Descriptive statistics of the physicochemical variables (n = 34 stations)

Variable	Min	Max	Mean	Std. dev.
NP (m)	1.210	52.700	23.862	14.520
T (°C)	18.290	22.530	20.894	1.082
Cond (µS/cm)	2.000	8408.000	1739.559	1751.435
Sal (g/L)	0.001	4.479	0.881	0.926
TDS (g/L)	0.001	5.633	1.165	1.174
H2O (g/L, water density)	997.700	1001.000	998.671	0.683
pH	6.743	6.828	6.782	0.022
O2 (mg/L)	6.777	7.717	7.243	0.242
%O2 (%)	84.360	93.250	89.079	2.795

deviation) of the nine physicochemical variables measured across the 34 sampling stations. These values provide the overall dataset context for the parameter-by-parameter analyses presented in the following subsections.

It is worth noting that H_2O (water density) values fall within a narrow, physically realistic range (997.7–1001.0 g/L), consistent with the known temperature dependence of pure water density; this consistency supports the internal validity of the field-measurement dataset as a whole.

The pronounced difference between the standard deviation of EC (1751.4 µS/cm), salinity (0.926 g/L), and TDS (1.174 g/L) relative to their means further illustrates the strong spatial heterogeneity in groundwater mineralization already highlighted in Section 2, and is examined in detail per parameter below.

Electrical conductivity

EC is one of the most informative indicators of groundwater mineralization, reflecting the concentration of dissolved ionic species and the intensity of water–rock interactions within the aquifer. Consequently, EC provides valuable information on groundwater quality and the hydrogeochemical processes governing groundwater evolution.

The measured EC values exhibited considerable spatial variability across the study area, ranging from 2 µS cm^{-1} at station S6 to 8408 µS cm^{-1} at station S1 (Figure 3). This wide range indicates pronounced heterogeneity in groundwater mineralization. According to the Moroccan drinking water standard (NM 03.07.001), which recommends a maximum permissible value of 2700 µS cm^{-1}, groundwater from stations S1, S2, S3, S4, S20, and S29 exceeded the recommended limit, suggesting poor groundwater quality in these locations.

The observed spatial variability in EC may be associated with differences in groundwater residence time and the extent of water–rock interaction, whereby the progressive dissolution of minerals contained in the geological formations would increase the concentration of dissolved ions along the flow path. Localized agricultural activities could also contribute to groundwater mineralization through the infiltration of dissolved salts and fertilizers. It should be noted that, based on a single sampling campaign, these interpretations describe spatial associations rather than demonstrated mechanisms, since residence time, flow velocity, and land-use pressure were not independently measured in this study.

The spatial distribution map (Figure 4) shows higher electrical conductivity values concentrated in the eastern and central-eastern part of the study area, particularly around stations S1, S3, S4, and S20, while station S6 recorded the lowest value of the dataset (2 µS/cm).

Salinity

Groundwater salinity provides a further indicator of mineralization, complementing the information derived from electrical conductivity (EC) and total dissolved solids (TDS). In the Khemisset–Tiflet aquifer, salinity values displayed pronounced spatial variability, ranging from 0.001 g L^{-1} at station S6 to 4.479 g L^{-1} at station S1 (Figure 5). Notably, the highest salinity value coincided with the station recording the maximum EC,

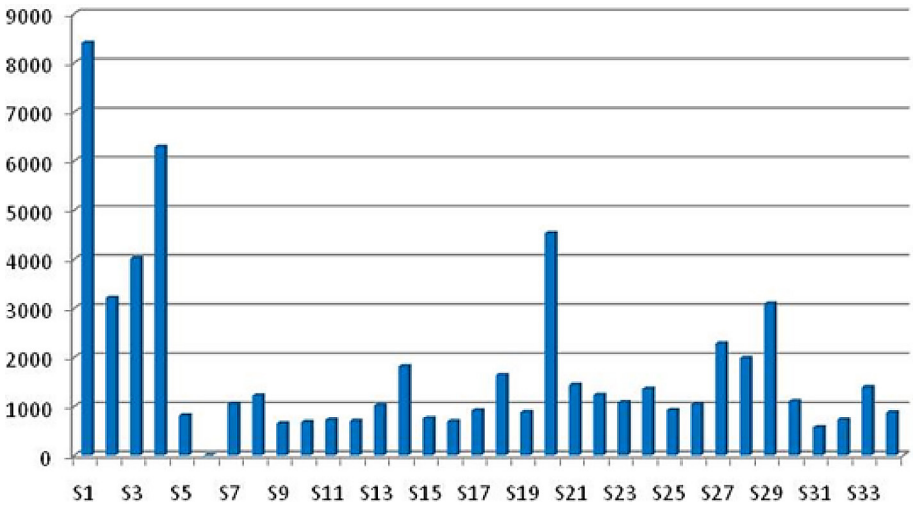

Figure 3. Variation of electrical conductivity across the sampling stations

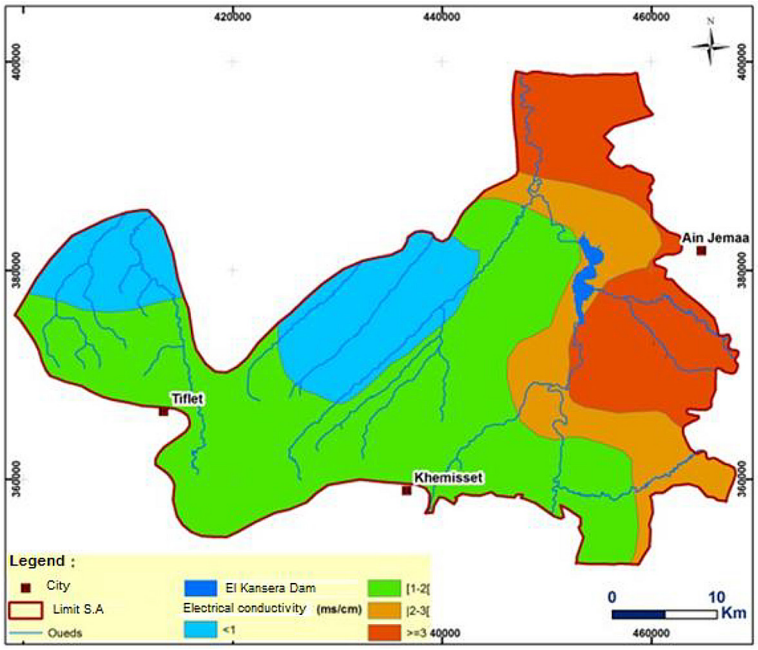

Figure 4. Spatial mapping of electrical conductivity in the study area

highlighting the close correspondence between salinity and the overall degree of groundwater mineralization.

As for EC, the spatial distribution of salinity shows a weak-to-moderate tendency toward higher values in the eastern and central-eastern sector, with values clustered around the same stations (S1, S3, S4, S20) rather than following a strict linear gradient. This pattern is broadly consistent with the regional groundwater-flow configuration inferred from the piezometric map.

The elevated salinity levels recorded at certain sampling locations may also be influenced by local hydrogeological and anthropogenic factors. Groundwater abstraction and agricultural practices, in particular, could affect the distribution of dissolved salts. However, the available dataset does not allow these contributions to be quantitatively distinguished from natural geochemical processes. The elevated salinity observed in the eastern sector should therefore be interpreted as the potential result of the combined influence of natural hydrogeochemical evolution and localized anthropogenic inputs.

A noteworthy field observation provides additional qualitative support for this interpretation. During the sampling campaign, well owners at sites characterized by high salinity, EC, and TDS

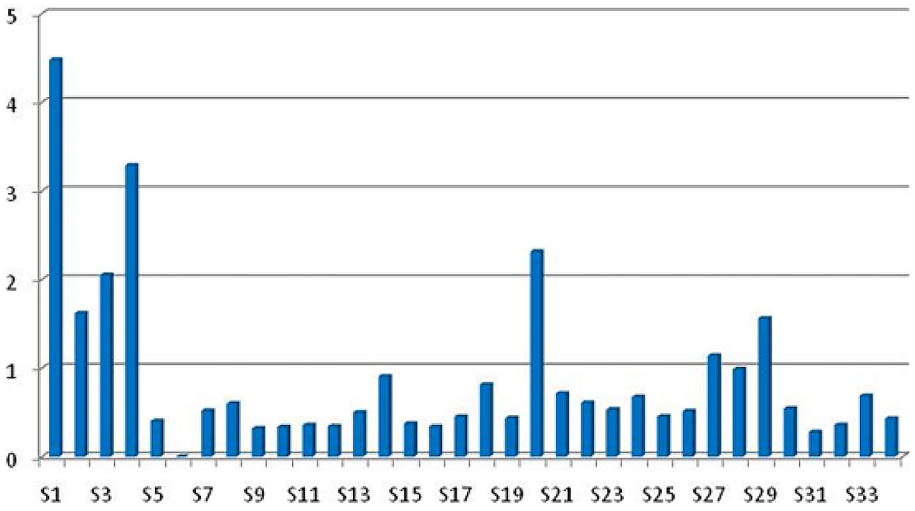

Figure 5. Spatial variation of groundwater salinity

reported a bitter taste in the groundwater. This observation was consistent with the analytical indication of increased mineralization and provides qualitative field evidence of the deterioration of groundwater characteristics at the most mineralized locations. Taken together, the salinity distribution confirms the pronounced spatial heterogeneity of groundwater mineralization within the Khemisset–Tiflet aquifer. The close correspondence among salinity, EC, and TDS indicates that these parameters largely capture the same mineralization gradient, while their spatial distribution points to the combined influence of groundwater flow, water–rock interaction, and potentially localized anthropogenic inputs.

Total dissolved solids

Total dissolved solids (TDS) represent the overall concentration of dissolved inorganic and organic constituents in groundwater and therefore provide an additional measure of its mineralization. In the Khemisset–Tiflet aquifer, TDS concentrations showed substantial spatial variability, ranging from 1 mg L^{-1} at station S6 to 5633 mg L^{-1} at station S1 (Figure 6), with an average value of 1165.12 mg L^{-1}.

The highest TDS concentration was recorded at station S1, which also exhibited the maximum electrical conductivity and salinity values. Conversely, station S6 recorded the lowest values for all three parameters. This close correspondence is supported by the Pearson correlation analysis, which yielded a correlation coefficient of r = 1.000 between TDS, EC, and salinity. These results indicate that the spatial variability of TDS is primarily associated with differences in the overall ionic content of groundwater and confirms the consistency of the three indicators as proxies for groundwater mineralization.

As for EC and salinity, TDS shows the same weak-to-moderate tendency toward higher values in the eastern/central-eastern sector, consistent by construction with the distributions observed for EC and salinity. Any progressive enrichment in dissolved solids along groundwater flow paths would be consistent with prolonged groundwater–rock interaction and increasing residence time.

The occurrence of elevated TDS values in some wells may also be influenced by local anthropogenic pressures, particularly groundwater abstraction and agricultural activities. However, these effects cannot be quantitatively separated from natural hydrogeochemical processes using the available dataset. Therefore, the observed TDS distribution should be interpreted as the result of the combined influence of natural groundwater evolution and potentially localized anthropogenic inputs.

Overall, the TDS results reinforce the evidence of strong spatial heterogeneity in groundwater mineralization within the Khemisset–Tiflet aquifer. The agreement among TDS, EC, and salinity strengthens the interpretation of an eastward increase in mineralization and provides a consistent basis for the subsequent multivariate analysis.

pH

The pH of groundwater is an important indicator of its acid–base conditions and can influence the mobility, dissolution, and precipitation of chemical

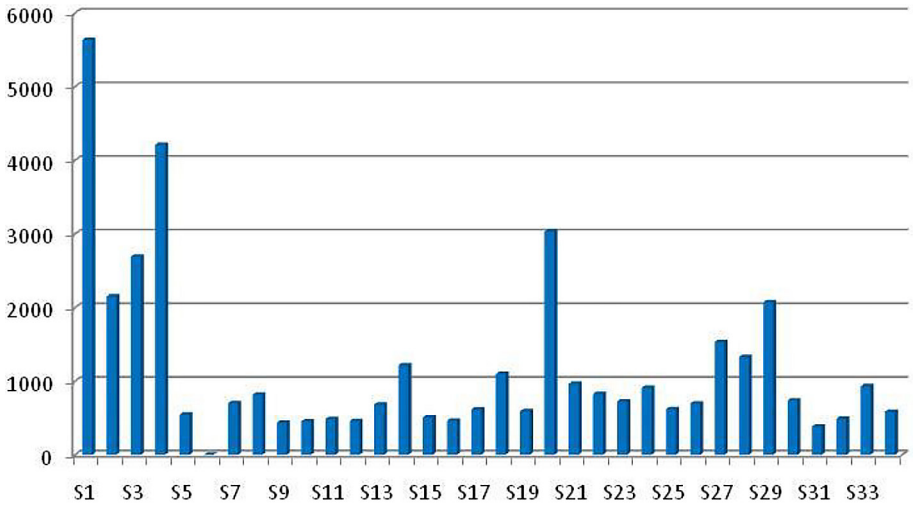

Figure 6. Variation of total dissolved solids (TDS) across the sampling stations

constituents within an aquifer. In the Khemisset–Tiflet aquifer, the measured pH values showed relatively limited variability, with an average value of 6.78 (Figure 7), indicating that groundwater was predominantly close to neutral conditions.

The relatively narrow variation in pH suggests that the groundwater system is characterized by generally stable acid–base conditions despite the marked spatial variability observed for mineralization-related parameters such as EC, salinity, and TDS. This contrast is noteworthy because EC, salinity, and TDS exhibited pronounced variability across the study area, whereas pH remained comparatively stable. The near-neutral pH conditions may be related to the buffering capacity of the aquifer system, particularly through interactions between groundwater and the geological formations encountered along groundwater flow paths. Mineral dissolution and carbonate-related reactions can contribute to maintaining groundwater pH within a relatively restricted range. However, the available dataset does not allow the contribution of individual buffering reactions to be quantified.

The Pearson correlation analysis also indicates relatively weak relationships between pH and the principal mineralization indicators, with correlation coefficients of 0.305 with EC, 0.303 with salinity, and 0.305 with TDS. This suggests that variations in groundwater mineralization are not directly accompanied by proportional changes in pH, supporting the interpretation that different processes control these two aspects of groundwater chemistry.

Overall, the pH results indicate that groundwater in the Khemisset–Tiflet aquifer remains generally close to neutral, while its mineralization varies considerably across the study area. This distinction between relatively stable acid–base conditions and highly variable mineralization provides an important basis for interpreting the subsequent hydrochemical and multivariate analyses.

Dissolved oxygen

DO is an important indicator of the redox conditions prevailing in groundwater and can provide information on the degree of groundwater interaction with the atmosphere and the intensity of biochemical processes within the aquifer. In the Khemisset–Tiflet aquifer, DO concentrations ranged from 6.777 to 7.717 mg L^{-1}, with an average value of 7.243 mg L^{-1} (Table 1, Figure 8).

Despite some spatial variability among sampling points, the relatively narrow range of measured DO concentrations indicates generally well-oxygenated groundwater during the sampling campaign. The observed concentrations may reflect the combined influence of atmospheric exchange during groundwater sampling, groundwater recharge conditions, temperature, and subsurface processes affecting oxygen consumption.

Temperature

Groundwater temperature is influenced by climatic conditions, groundwater depth, recharge processes, and the degree of interaction between groundwater and the surrounding geological formations. In the Khemisset–Tiflet aquifer, the measured groundwater temperatures ranged from 18.29 °C at station S25 to 22.53 °C at station S7 (Figure 9), with an average value of approximately 21 °C.

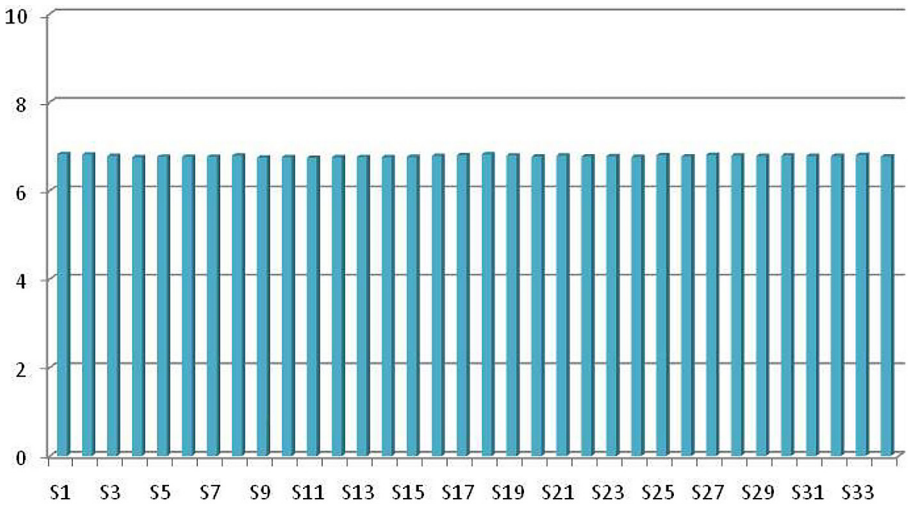

Figure 7. Variation of pH across the sampling stations

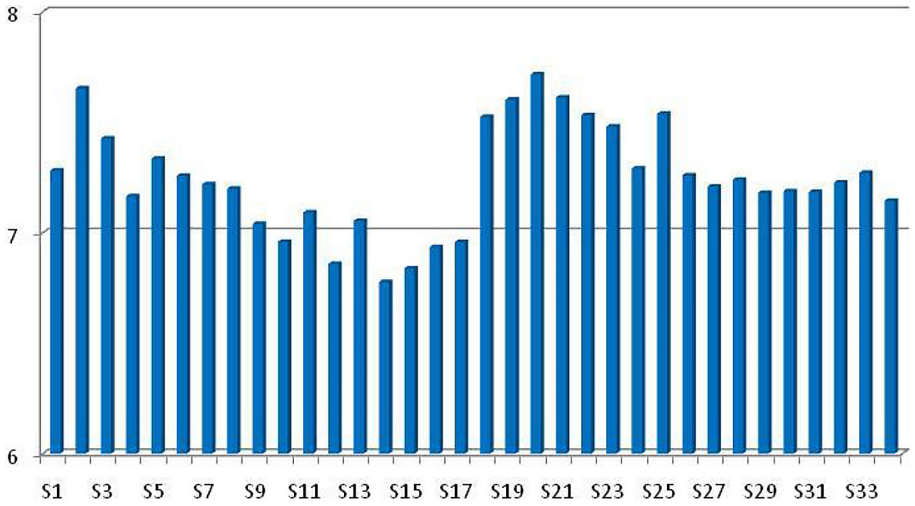

Figure 8. Distribution of dissolved oxygen across the sampling stations

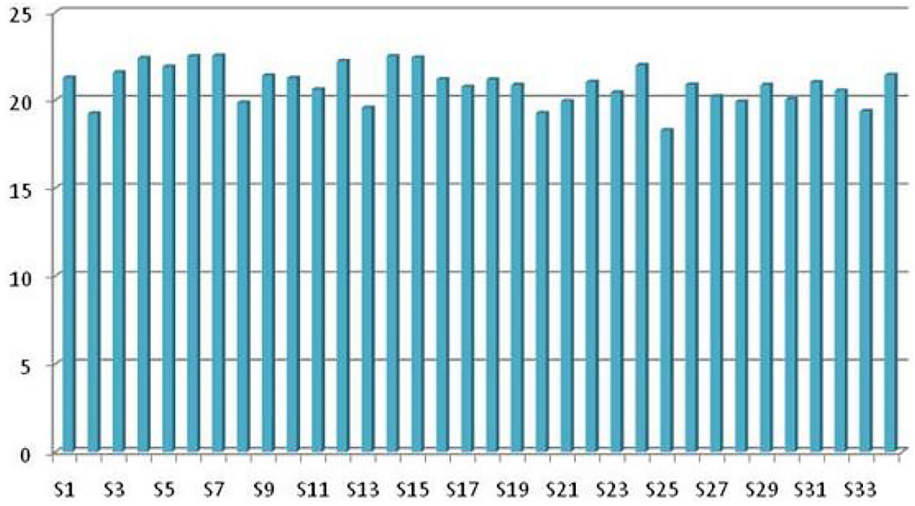

Figure 9. Variation of groundwater temperature across the sampling stations

The relatively limited temperature range observed among the sampling sites suggests generally homogeneous thermal conditions within the investigated groundwater system during the May 2018 sampling campaign. The observed spatial variability may partly reflect differences in well depth, local recharge conditions, and the degree of connection between groundwater and near-surface processes. However, the available dataset does not allow the individual contribution of these factors to be quantified.

The temperature distribution also shows no strong relationship with the main indicators of groundwater mineralization. Pearson correlation coefficients between temperature and EC, salinity, and TDS are relatively low ($r = 0.191$, 0.187, and 0.191, respectively), indicating that the spatial variability of groundwater temperature is largely independent of the mineralization gradient. Overall, groundwater temperature remained relatively stable across the study area during the sampling period. Its limited variability and weak association with EC, salinity, and TDS indicate that temperature does not appear to be a major factor controlling the spatial distribution of groundwater mineralization in the investigated aquifer.

Piezometric distribution and groundwater flow

The piezometric map is of critical importance for characterizing aquifer systems, as it provides information on the hydrodynamic behavior of the groundwater body and on reservoir functions,

including flow direction, hydraulic gradients, drainage by rivers, and zones subject to intensive groundwater abstraction. It offers an instantaneous representation of the state of the aquifer at a given point in time. The piezometric level corresponds to the elevation of the water level in natural equilibrium within the well; it constitutes the upper boundary of the water table within the aquifer — a hydrodynamic limit that can rise or fall freely within the permeable hydrogeological formation. It is calculated as the difference between the ground-surface elevation at the well (reference elevation, Z) and the depth to water (NP).

The spatial distribution of groundwater levels was investigated using the piezometric measurements collected during the May 2018 sampling campaign. At each station, the depth to the groundwater level below ground surface (NP) was measured using a water-level probe, and the ground-surface elevation (Z) was determined by GPS together with the X and Y geographic coordinates of the well. NP ranged from 1.21 to 52.70 m (mean = 23.86 m; Table 1). To construct the piezometric map, these depths were converted into hydraulic head elevations (in meters above sea level) by subtracting NP from Z at each well. The resulting piezometric map (Figure 10) shows a marked spatial variability in groundwater head elevation across the Khemisset–Tiflet aquifer, with equipotential values ranging approximately from 100 to 400 m a.s.l.

The configuration of the equipotential lines indicates a general groundwater flow from areas of higher hydraulic head toward areas of lower hydraulic head. The groundwater flow directions, represented by the flow arrows on the piezometric map, show a predominantly southwestern to northeastern and southern to northeastern flow pattern, with groundwater converging toward the central-eastern part of the study area.

The observed piezometric configuration provides an important framework for interpreting the spatial distribution of groundwater quality parameters. In particular, the areas characterized by lower electrical conductivity, salinity, and TDS are mainly located in the western and central-western sectors, whereas higher mineralization occurs predominantly toward the eastern part of the study area. This spatial organization suggests that groundwater chemistry evolves along the flow system and may progressively change as groundwater circulates through the aquifer.

The increase in mineralization along groundwater flow paths may be associated with increasing groundwater–rock interaction and residence time. During groundwater circulation, contact with the geological formations can promote the dissolution of minerals and the accumulation of dissolved constituents. However, the observed mineralization pattern may also be influenced by spatial variations in lithology, recharge conditions, groundwater abstraction, and agricultural

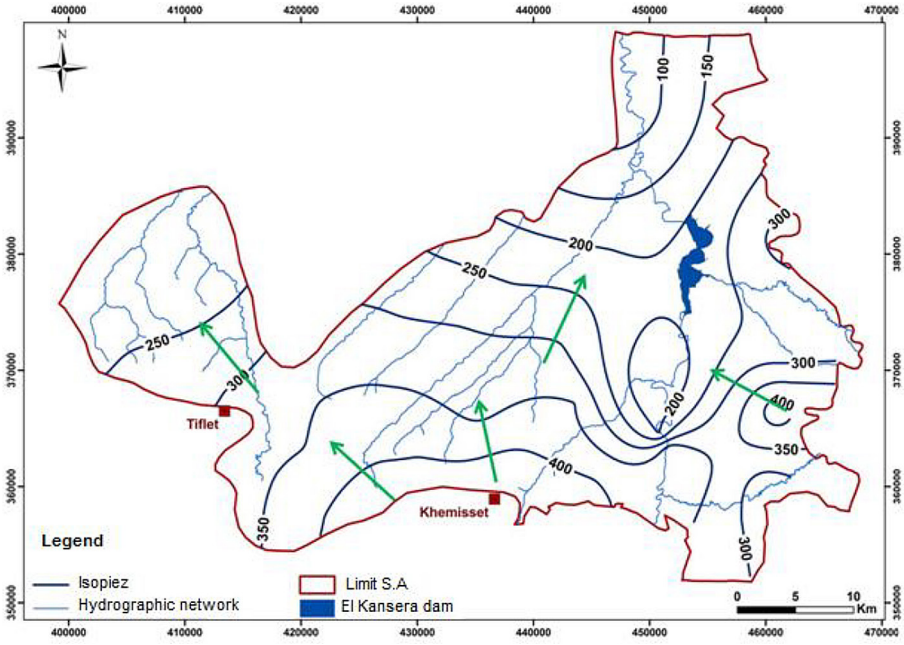

Figure 10. Piezometric map with groundwater flow direction

activities. The present dataset does not allow the relative contribution of these processes to be quantified independently.

The integration of the piezometric and hydrochemical maps therefore suggests that groundwater flow is an important factor to consider when interpreting the spatial distribution of groundwater mineralization. The combination of hydraulic and hydrochemical information provides a more comprehensive understanding of groundwater evolution within the Khemisset–Tiflet aquifer. This relationship is further investigated through the multivariate statistical analysis presented in the following section.

Major and trace elements

Complementary laboratory analyses of major and trace elements were performed for a subset of seven sampling stations (S1, S4, S13, S17, S20, S29, and S33), selected among the sites exhibiting the highest levels of mineralization. Figure 11 illustrates the concentrations of calcium (Ca), sodium (Na), magnesium (Mg), aluminum (Al), chromium (Cr), iron (Fe), manganese (Mn), and phosphorus (P) across these stations.

Sodium, calcium, and magnesium were the most abundant constituents, with average concentrations of 267.16, 137.78, and 49.70 mg/l, respectively. Station S1 recorded the highest concentrations of both sodium (767.42 mg/l) and calcium (244.66 mg/l), which is consistent with the elevated TDS, electrical conductivity, and salinity values previously recorded at this station, confirming that Na+ and Ca2+ constitute the dominant ionic species driving groundwater mineralization at this site. Aluminum, chromium, iron, and manganese were present at comparatively lower and more uniform concentrations across the seven stations, while phosphorus levels remained consistently low (< 0.7 mg/l) at all sites.

The correspondence between the elevated Na and Ca concentrations at station S1 and its already-identified maximum EC, TDS, and salinity values provides direct chemical confirmation of the mineralization patterns inferred from the physicochemical parameters, and further supports the interpretation of water–rock interaction as the dominant process controlling groundwater chemistry in the most mineralized sector of the aquifer.

Principal component analysis

The Pearson correlation matrix revealed very strong positive relationships among electrical conductivity, salinity, and TDS, with pairwise correlation coefficients of 1.000, confirming that these three parameters describe the same mineralization signal. Strong positive correlations were also found between water density (H2O) and EC (r = 0.937), salinity (r = 0.933), and TDS (r = 0.937), consistent with the physical expectation

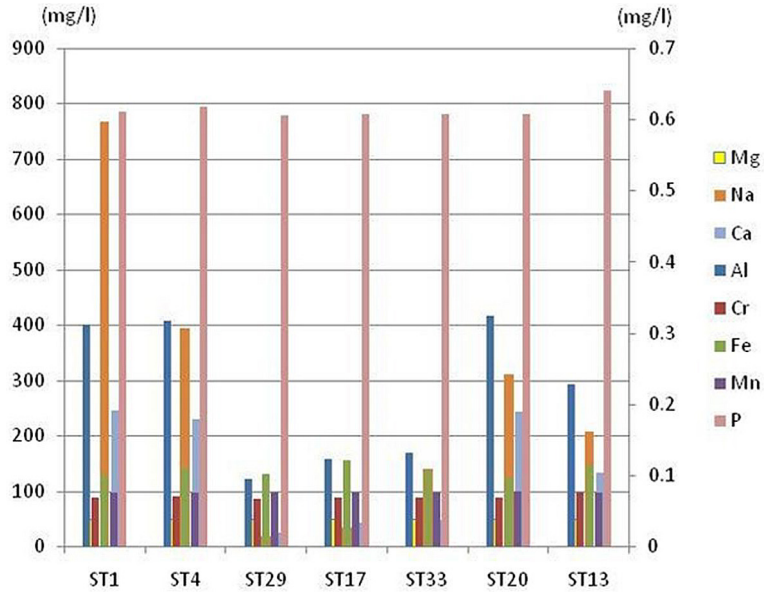

Figure 11. Variation of major and trace element concentrations (Ca, Na, Mg, Al, Cr, Fe, Mn, P) at selected sampling stations

that dissolved-solid content increases water density. In contrast, pH showed comparatively weak correlations with EC, salinity, and TDS ($r \approx 0.30$), and dissolved oxygen displayed similarly limited associations with the mineralization-related parameters (Table 2).

The PCA was run on the nine standardized active variables defined in Section 2.3 and therefore extracted nine principal components in total, whose eigenvalues sum to 9.000 by construction. Table 3 reports all nine components; the first two (F1 and F2) accounted for 76.9% of the total variance (F1 = 53.6%, F2 = 23.3%), and the first four components together accounted for 97.5% of the total variance, indicating that most of the variability in the physicochemical dataset can be summarized along these axes, while components F6–F9 each contributed less than 0.02% and are not further interpreted.

As shown in Table 4, the F1 axis was strongly and positively defined by water density H2O (r = 0.970), electrical conductivity (r = 0.910), TDS (r = 0.910), and salinity (r = 0.906), confirming that this axis primarily represents the groundwater mineralization gradient; the strong loading of water density on this same axis is physically consistent with the expected increase in water density with dissolved-solid content. The F2 axis, by contrast, was mainly defined by temperature (r = 0.861) and depth to groundwater NP (r = 0.624), and only very weakly by water density (r = 0.058), indicating that this second dimension reflects processes distinct from mineralization — likely related to recharge conditions and thermal variability across the aquifer.

The factorial representation (Figures 12 and 13) provides a graphical synthesis of these relationships, distinguishing sampling sites according to their degree of mineralization along F1 and their thermal/piezometric characteristics along F2. This structure is consistent with the spatial distributions observed for EC, salinity, and TDS, which show higher mineralization toward the eastern part of the study area, and reinforces the interpretation that groundwater mineralization constitutes the principal dimension of variability within the physicochemical dataset, while a secondary, largely independent dimension is associated with temperature and hydraulic head.

Table 4. Correlations between the physicochemical variables and the first three principal components

Variables	F1	F2	F3
NP	-0.606	0.624	0.254
T	-0.336	0.861	0.223
Cond	0.910	0.388	-0.143
Sal	0.906	0.396	-0.146
TDS	0.910	0.388	-0.143
H2O	0.970	0.058	-0.205
pH	0.559	-0.509	0.008
O2	0.565	-0.467	0.660
%O2	0.542	0.174	0.818

Table 2. Pearson correlation matrix of the physicochemical parameters

Variables	NP	T	Cond	Sal	TDS	H2O	pH	O2	%O2
NP	1								
T	0.743	1							
Cond	-0.339	-0.010	1						
Sal	-0.333	-0.001	1.000	1					
TDS	-0.339	-0.010	1.000	1.000	1				
H2O	-0.586	-0.357	0.937	0.933	0.937	1			
pH	-0.524	-0.502	0.305	0.303	0.305	0.461	1		
O2	-0.465	-0.489	0.241	0.233	0.242	0.403	0.467	1	
%O2	-0.047	0.165	0.442	0.440	0.442	0.363	0.203	0.762	1

Table 3. Eigenvalues and explained variance of all nine principal components (sum of eigenvalues = 9.000)

Parameter	F1	F2	F3	F4	F5	F6	F7	F8	F9
Eigenvalue	4.824	2.099	1.324	0.529	0.221	0.002	0.001	0.000	0.000
Variability (%)	53.602	23.323	14.707	5.883	2.453	0.017	0.011	0.003	0.000
Cumulative (%)	53.602	76.925	91.632	97.515	99.968	99.986	99.997	100.000	100.000

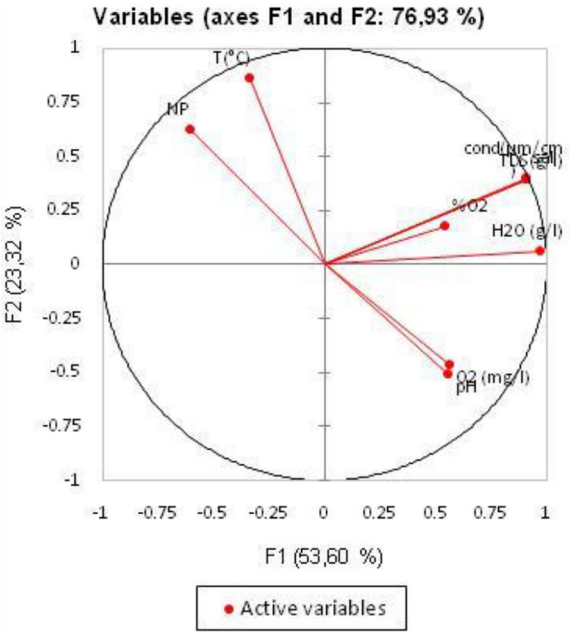

Figure 12. Correlation circle of the physicochemical variables (PCA)

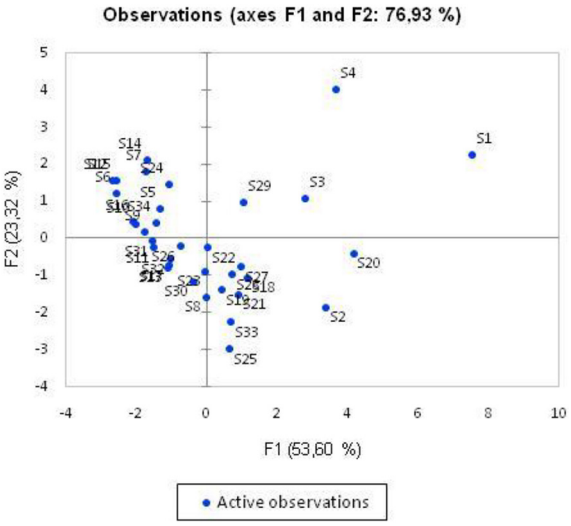

Figure 13. Factorial map of the sampling stations (PCA)

CONCLUSIONS

This study investigated the spatial distribution and hydrochemical characteristics of groundwater in the Khemisset–Tiflet area using an integrated approach combining field measurements, laboratory analyses, hydrochemical interpretation, spatial mapping, and multivariate statistical analysis. A total of 34 groundwater samples were investigated during the May 2018 sampling campaign, providing a spatially distributed dataset for assessing groundwater quality and mineralization patterns. The results revealed marked spatial variability in groundwater physicochemical characteristics. Electrical conductivity, salinity, and TDS showed consistent spatial variations, with the highest mineralization levels concentrated in specific sectors of the study area, particularly in its eastern part. Several sampling sites exceeded the Moroccan guideline value for electrical conductivity, indicating elevated mineralization in localized sectors of the study area. The strong correlation observed among EC, salinity, and TDS further indicates that these parameters describe a common mineralization signal.

The spatial distribution of the physicochemical parameters, considered together with the piezometric configuration, suggests that groundwater circulation and water–rock interaction may contribute to the observed hydrochemical variability. Potential anthropogenic influences, particularly those associated with agricultural activities and groundwater abstraction, may also contribute to the observed spatial heterogeneity. Given the available dataset, the relative contribution of natural and anthropogenic processes cannot be quantitatively separated. These interpretations are based on a single sampling campaign conducted in May 2018 and therefore represent spatial associations rather than demonstrated mechanisms; seasonal and interannual variability could not be assessed.

The multivariate analysis provided complementary information on the relationships among the physicochemical parameters. The PCA highlighted the strong association between EC, salinity, and TDS and identified a secondary dimension of variability linked mainly to temperature and piezometric level. These results highlight the importance of the mineralization gradient in structuring the physicochemical variability of groundwater in the study area. It should be noted that EC, salinity, and TDS are strongly interrelated parameters in multiparameter probe measurements; therefore, their strong contribution to this mineralization axis primarily reflects a common mineralization signal rather than independent sources of variability.

Complementary ICP-AES analyses were performed on seven pre-selected highly mineralized stations. These analyses provided additional information on the elemental composition of the most mineralized groundwater samples; however, their restricted and non-random sampling coverage prevents extrapolation of these results

to the entire aquifer. Overall, the integrated hydrochemical and spatial approach provides a baseline characterization of groundwater quality in the relatively poorly documented Khemisset–Tiflet aquifer. The spatial interpolation based on 34 sampling points should be interpreted as indicative of broad spatial trends rather than as a fully validated continuous surface. The results emphasize the need for continued groundwater-quality monitoring, particularly in the most mineralized sectors, together with improved monitoring of groundwater abstraction and agricultural activities.

In particular, the major anions (HCO_3^-, SO_4^{2-}, Cl^-, NO_3^-, etc.) were not analyzed in the present study. Their systematic measurement in future campaigns would enable ionic-balance calculations and formal hydrochemical facies classification, thereby improving the qualitative and quantitative understanding of groundwater characteristics and hydrochemical processes in this relatively poorly documented aquifer. Future investigations combining denser temporal sampling and systematic major- and trace-element analyses across a representative, rather than pre-selected, set of stations would further help distinguish natural geochemical processes from anthropogenic influences and improve the assessment of groundwater vulnerability.

Finally, station S6, which recorded an exceptionally low EC value, warrants dedicated investigation in future sampling campaigns. Complementary hydrogeochemical and isotopic approaches, including stable water isotopes and sampling of nearby surface water, could help test whether local surface-water/groundwater interactions contribute to this unusual observation.

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