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Drinking water quality assessment using water quality index: A case study of the Shahrekord, Iran

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ABSTRACT

In recent years, the use of water quality indices (WQI) to ensure the safety of drinking water has expanded. In this study, the quality of drinking water in Shahrekord was investigated. This study involves measuring eight physicochemical parameters (pH, EC, TDS, TH, SO_4^{2-}, PO_4^{3-}, NO_3^-, Turbidity) of drinking water taken from the urban water network and calculating the water quality index. The obtained water quality index obtained for all water samples was below 50, indicating excellent and very good quality of Shahrekord's drinking water. After applying principal component analysis, the results indicated that first component, with the highest eigenvalue, is influenced by parameters such as sulfate, nitrate, electrical conductivity (EC), and TDS, confirming the salinity and chemical water quality are dominant. The second component, driven by phosphate, total hardness (TH), and turbidity, reflects the physical properties and hardness of water. The third component is associated with the contribution of phosphate and hardness. EC and TDS exhibit a high correlation.

1. Introduction

Water is an irreplaceable necessity for human survival. Currently, over one billion people in the world lack access to safe drinking water. It is predicted that in the coming years, the number of countries facing water scarcity will increase to two-thirds. Nearly 80% of consumed water is returned to the environment untreated [1]. Environmental pollution, declining water quality, and reduced access to freshwater are among the consequences. In recent years, to mitigate these damages, the World Health Organization (WHO) and the European Union have established guidelines to improve water quality and promote proper environmental management [2]. Today, to ensure drinking water quality, permissible limits are defined for various physical, chemical, and microbiological parameters. However, these values alone cannot fully represent water quality. Therefore, using a comprehensive index that accounts for the combined effects of all these factors was proposed as a practical solution. Experts subsequently introduced an index called

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the WQI [3]. The WQI is used to simplify and facilitate rapid, accurate interpretation of drinking water test results. This index can also be customized based on regional conditions (water sources and end-users). The first WQI model was introduced by Horton in 1960, based on ten water quality parameters. Later, the U.S. National Sanitation Foundation (NSF) developed the NSFWQI model. Researchers have developed more than 35 WQI models, each with its own distinct advantages and limitations [4]. The selection of an appropriate model depends on regional conditions, local guidelines, and data availability. By evaluating existing research studies, it can be concluded that the most important parameters used in water quality indices include [5]: Ammonia (NH_3), Calcium (Ca), Chloride (Cl), Electrical Conductivity (EC), Fluoride (F), Hardness ($CaCO_3$), Magnesium (Mg), Manganese (Mn), Nitrate (NO_3), pH, Sulfate (SO_4), and Turbidity (Turb). The Water Quality Index (WQI) is formulated based on the following four stages of selection of water quality parameters, determination of parameter sub-indices, assignment of parameter weights, aggregation of sub-indices to calculate the overall water quality index, and selection of Water Quality parameters [6].

The determination of the number of selected parameters in the water quality index calculation process is performed using supervised and unsupervised classification algorithms, statistical ranking-based techniques, and a combination of both methods [7].

Since the parameters used in the water quality index have different measurement units, sub-indices are employed to convert the results to a dimensionless scale. To determine sub-indices, methods such as expert judgment, water quality standards, and statistical approaches are utilized [8].

The assigned weight for each parameter is a function of its relative importance to overall water quality. While some models assign equal weights to all parameters, most water quality index models employ differential weighting based on each parameter's significance [9]. The cumulative weight of all quality parameters must not exceed 100% [10]. Improper parameter weighting will compromise the index's validity, rendering the final WQI value unrepresentative of actual water quality [11]. The Delphi method and Analytic Hierarchy Process (AHP) are employed for parameter weighting [12]. The Delphi method relies on collecting expert opinions, statistical summarization, and iterative repetition of the process until consensus is achieved [13]. In this method, researchers assign parameter weights based on available data using 1-to-5 or 1-to-4 rating scales to compare the environmental significance of different factors. To derive relative weights ranging from 0 (least impact) to 1 (greatest impact), all scores are aggregated, and their arithmetic means are either calculated through mathematical functions or compared against existing standards. Assessing the water quality of the provincial capital, providing a perspective on water quality and the status of physicochemical parameters of drinking water, and analyzing trends or combining them with statistical tools such as PCA to extract parameter relationships and interpret the results are among the features of this research.

This study involves measuring eight physicochemical parameters (pH, EC, TDS, TH, SO_4^{-2}, PO_4^{3-}, NO_3^-, Turbidity) of water in ten samples from the urban water network and calculating the water quality index. Following the calculation of the Water Quality Index (WQI) for Shahrekord, Principal Component Analysis (PCA) was used to interpret the results, examine the relationships between variables, and uncover hidden patterns.

2. Materials and methods

2.1. Study Area

In this study, the municipal water of Shahrekord, the capital of Chaharmahal and Bakhtiari province in Iran, was investigated. Chaharmahal and Bakhtiari, with an area of 16,532 square kilometers, is located in the southwest of Iran, in the center of the Zagros Mountains. The provincial capital, Shahrekord, is situated at an altitude of 2,066 meters above sea level, making it the highest provincial capital in Iran. The geochemical mapping, ArcGIS 10.5 was used to obtain the map of the studies area. The geographical location of Shahrekord is shown in Figure 1. The two main sources of water for the city of Shahrekord are the

Koohrang water transmission line and the Ben–Borujen water transmission line. The Koohrang water transmission line transfers water from the Dimeh and Koohrang springs to Shahrekord. The Koohrang region is part of the Central Zagros, and its hydrogeology is primarily based on karst aquifers in the carbonate (limestone) rocks of the Zardkooh range. These aquifers are recharged both at the surface and subsurface mainly by snowmelt and winter precipitation on Zardkooh.

The area along the transmission line route (from Ben to Borujen) is also part of the Central Zagros, and its hydrogeology is influenced by the Zayandeh-Rud drainage basin. The aquifer type in this section is alluvial–limestone.

2.2. Water sampling

Sampling from the water distribution network of Shahrekord was conducted according to the Iranian National Standard No. 7002 (First Revision) from ten points across the city, taking into account geographical distribution, low-pressure zones, endpoints of the network, and other standard requirements. Eight physicochemical parameters related to 10 water samples from across Shahrekord were measured.

2.3. Determination of properties of water

In this research, standard methods were used to measure certain physicochemical parameters of water (pH, EC, TDS, TH, SO_4^{2-}, PO_4^{3-}, NO_3^-, Turbidity) for the purpose of determining the Water Quality Index (WQI).

2.4. Calculation of WQI:

To determine the Water Quality Index (WQI), the set of the relative weight (Wi), Quality Rating Scale (qi), Sub-index of Water Quality (SIi), and Overall Water Quality Index (WQI) including equations (1) to (4) were used as follow [14,15]:

$$W_i = w_i/\sum(w_i) \tag{1}$$

$$q_i = (C_i S_i) \times 100 \tag{2}$$

$$SI_i = W_i \times q_i \tag{3}$$

$$WQI = \sum(SI_i) \tag{4}$$

In which:

Wi: Relative weight of water quality parameters.

qi: Quality score for each parameter, based on the ratio of observed concentration (Ci*Ci*) to the standard (Si*Si*).

SIi: Sub-index of water quality for each parameter.

WQI: Final water quality index, obtained from the sum of all sub-indices.

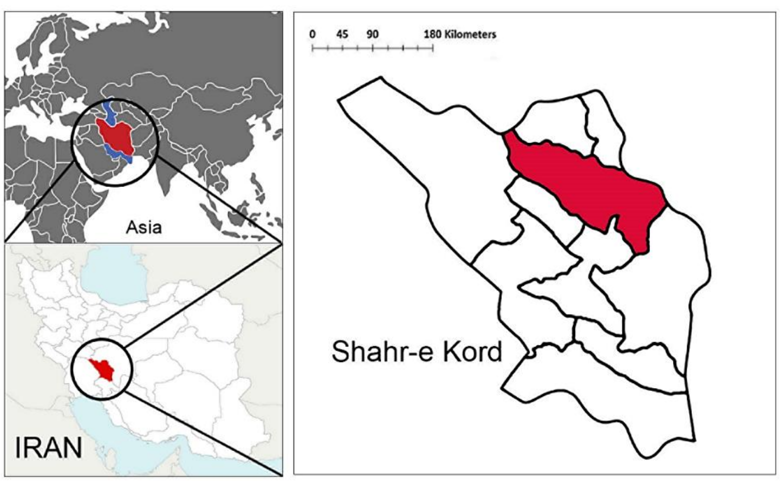

Fig. 1. The map of monitoring station

The table below presents 8 measured parameters from 10 water samples, along with the corresponding limits from the Iranian National Standard 1053 (Sixth Revision), measurement units, assigned weights for each parameter, and the relative weight of each variable (Table 1). The WQI standard data based on WHO is tabulated in Table 2 [15].

2.5. Principal component analysis (PCA)

Multivariate statistical analysis comprises a set of techniques designed to reduce initial data dimensions ,identify common trends, provide an interpretable overview of relationships between parameter [16] .PCA is one of the most widely used multivariate analysis methods, employed to: Reduce a large number of initial variables into a limited set of principal components (PCs) [17]. Extract weighted linear combinations of variables that capture the most significant parameters while representing the entire dataset. Reduce data volume by interpreting variability across results.
This level of analysis cannot be achieved through simple correlation methods. In Principal Component Analysis (PCA), the variance of the linear combination of parameters is maximized by finding the optimal weights [18].

3. Results and discussion

3.1. WQI

Using standard methods, the physicochemical parameters of water samples from Shahrekord were measured. By comparing the obtained values with standard limits, it can be stated that the parameter values did not exceed the permissible limits and are acceptable (Table 3).

Table 1. Water Quality Parameters and Assigned Weights

Parameter	Standard	Unit	w_i	W_i
pH	6.5-8.5	-	4	0.125
EC	1500	µmhos/cm	4	0.125
TDS	1000	mg/L	5	0.15
TH	300	mg/L	3	0.093
SO_4^{-2}	250	mg/L	4	0.125
PO_4^{3-}	5	mg/L	4	0.125
NO_3^-	50	mg/L	5	0.15
Turbidity	1	NTU	3	0.093

Table 2. Water Quality Index (WQI) Classification [15]

status	WQI
Excellent	<50
Good	50-100
Poor	100-200
Very poor	200-300
Water unfit for drinking	> 300

Table 3. The measured values of parameters in water samples from Shahrekord.

Sample	pH	SO_4^{2-}	TDS	TDS	PO_4^{3-}	Turbidity	NO_3^-	EC
1	7.63	47.18	353.22	138.14	0.026	0.12	16.70	517
2	7.84	13.39	157.88	122.79	0.025	0.11	0.01	218
3	7.99	18.44	203.98	120.72	0.077	0.17	0.01	303
4	7.95	18.18	184.70	88.09	0.024	0.15	4.05	295
5	7.82	4.33	162.48	134.97	0.033	0.19	5.26	228
6	7.79	22.20	200.68	252.24	0.031	0.23	6.72	298
7	7.86	13.39	163.78	214.98	0.037	0.05	3.62	233
8	7.75	15.33	252.92	120.09	0.026	0.07	7.50	362
9	8.02	14.17	133.22	127.89	0.027	0.10	4.05	217
10	7.92	18.05	201.36	27.67	0.025	0.12	1.21	303

After determining the weights of the parameters, the Water Quality Index (WQI) of Shahrekord was calculated. The individually measured parameters showed that all values were within acceptable and standard limits. None of the key parameters affecting the WQI exceeded the standard limits. Naturally, the overall water quality, reflected by the WQI values in the excellent to very good range, confirmed the high quality of the samples. The reliable water sources supplying Shahrekord's urban network ensure its high quality. The results, below 50, indicated that according to water quality classification, the water falls within the "excellent to very good" range (Table 4).

3.2. PCA

As shown in Table 5 and Table 6, the table of eigenvalues for the correlation matrix, information such as eigenvalues, the proportion of each component's contribution to the total variance of the data, and the cumulative variance is provided. For the number of principal components (eight components), eight eigenvalues are reported, which describe the amount of variance explained by each component. Higher eigenvalues indicate a greater contribution to the variance. Components 1 to 4 have the highest eigenvalues and, consequently, the greatest impact, while components 5 to 8, with eigenvalues less than one, are of lesser importance. The proportion of variance explained (Proportion) indicates each component's share of the total variance. For example, PC1 alone accounts for more than 50% of the variance. The cumulative variance (Cumulative) describes the total variance explained up to that point. The first four components (PC1 to PC4) cover more than 93% of the variance, indicating nearly complete coverage of the data's information.

Table 4. The calculated Water Quality Index (WQI) results

Samples	WQI	Quality of water
1	33.51	Excellent and very good
2	21.91	Excellent and very good
3	23.72	Excellent and very good
4	23.11	Excellent and very good
5	23.63	Excellent and very good
6	29.97	Excellent and very good
7	24.82	Excellent and very good
8	22.60	Excellent and very good
9	22.40	Excellent and very good
10	20.43	Excellent and very good

Table 5. Eigen analysis of the Correlation Matrix

Eigenvalue	4.2358	1.3756	1.1733	0.7273	0.3161	0.1356	0.0363	0.0001
Proportion	0.529	0.172	0.147	0.091	0.040	0.017	0.005	0.000
Cumulative	0.529	0.701	0.848	0.939	0.979	0.995	1.000	1.000

Table 6. The Eigenvectors of variables

Variable	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8
pH	-0.407	-0.035	0.342	0.002	-0.665	0.320	-0.369	0.187
SO4	0.431	0.054	0.218	0.038	-0.611	-0.464	0.417	-0.006
TDS	0.465	-0.002	0.233	0.055	0.212	-0.056	-0.348	0.747
TH	0.057	0.557	-0.595	0.411	-0.234	-0.101	-0.314	0.034
PO4	-0.123	0.519	0.553	0.500	0.246	0.160	0.263	-0.066
Turbidity	-0.018	0.645	0.084	-0.758	0.027	-0.020	-0.021	0.024
NO3	0.449	0.029	-0.195	-0.042	-0.153	0.800	0.305	0.030
EC	0.460	-0.012	0.279	0.004	0.015	0.048	-0.555	-0.633

PC1, with the highest eigenvalue, is influenced by parameters such as total dissolved solids, electrical conductivity, nitrate, sulfate, and pH indicating that chemical water quality is dominant. The second component, with a high influence from, Turbidity, total hardness, and phosphate, reflects the physical properties and hardness of water. The third component is associated with the contribution of total hardness and phosphate.

The PCA outlier detection plot with a critical line at 43.72 indicates that none of the observations are outliers (Figure 2), and the data are uniformly distributed around the mean, with no observation unusually separated from the others. The scree plot is a graph that displays eigenvalues against component numbers (Figure 3), allowing the selection of an appropriate number of principal components for data analysis.

At the elbow point, the eigenvalues significantly decrease, and subsequent components contribute little additional variance. The main elbow point occurs between the third and fourth components, indicating that the first three principal components account for the majority of the variance. The results of this plot are fully consistent with the eigenvalue table. The score plot displays observations in the space between the first and second principal components, allowing evaluation of the sample distribution pattern (Figure 4).

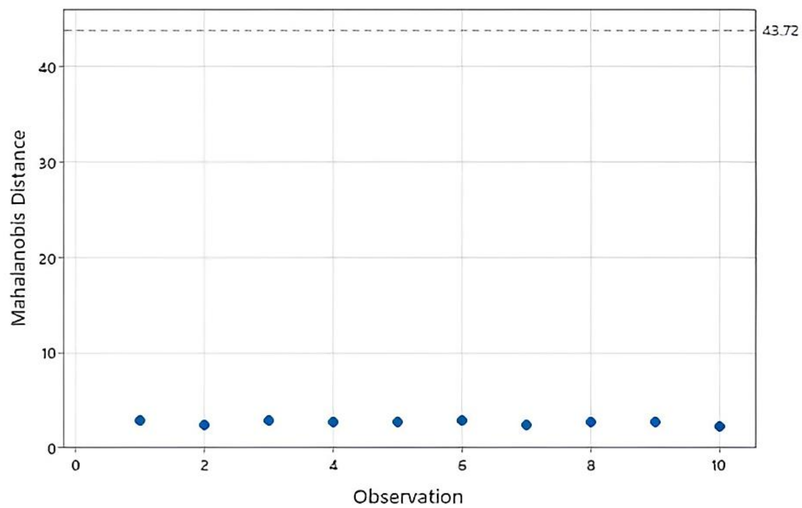

Fig. 2. The PCA outlier detection plot

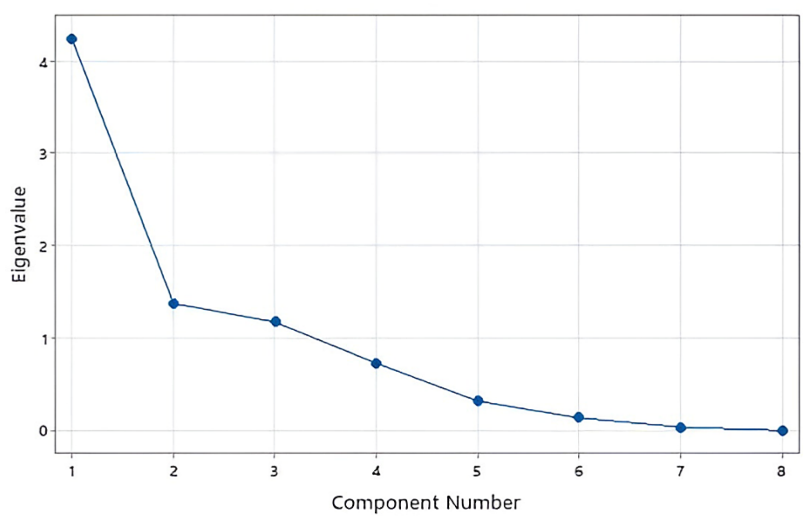

Fig. 3. The PCA scree plot

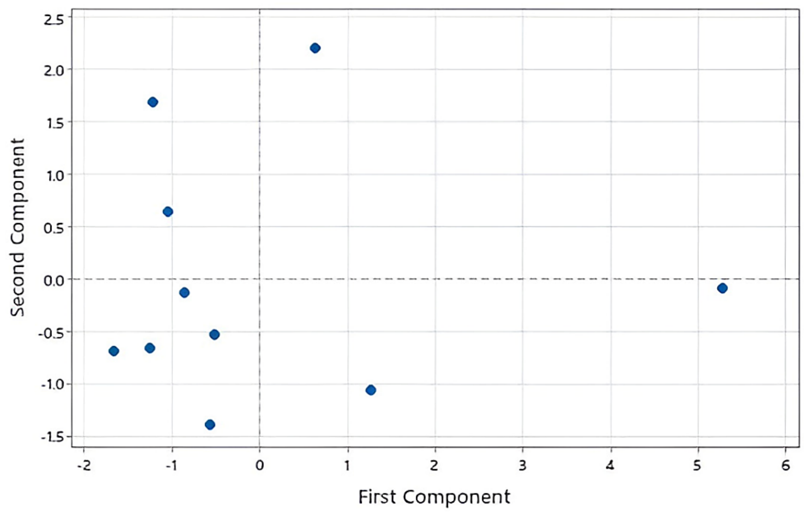

Fig. 4. The PCA score plot

Component scores are based on eigenvalues and variance contributions. The plot shows no outliers, with greater dispersion along the first component, consistent with its higher variance. The plot also provides a clustering perspective, where similar samples are closer together. Waters with higher salinity or hardness are grouped in one cluster.

The loading plot reflects the relationship between principal components and variables, as well as the correlation between variables (Figure 5).

Data points for variables are displayed in the space between the two principal components with the highest variance contributions. Normalized scales from -1 to +1 indicate the weight of each variable in the components.

Variables such as sulfate, nitrate, electrical conductivity (EC), and TDS in the positive section of PC1 show a strong relationship with the first principal component.

Variables close to each other on the plot, such as EC and TDS in PC1, and PO4, total hardness (TH), and turbidity in PC2, exhibit high correlation. Variables positioned in opposite directions, such as pH on the negative side and EC/TDS on the positive side, have a negative correlation.

The biplot simultaneously displays the scores of observations and the loadings of variables in the space of the two principal components that account for the most variance (Figure 6).

This plot combines the score plot and loading plot, enabling a visual interpretation of the relationship between samples and variables.

The points on the plot represent observations or samples, while the direction and length of the arrows indicate the direction and strength of the variables' influence on the first and second components.

In this biplot, the long arrows for sulfate, nitrate, electrical conductivity (EC), and TDS with a positive orientation demonstrate their strong influence on the first component. The negative direction of pH relative to the first component indicates an inverse relationship with the other parameters of the first component.

Turbidity, total hardness (TH), and phosphate have a strong influence on the second principal component. EC and TDS show high correlation. Sample 1 is close to TDS/EC, and sample 6 is close to Turbidity/TH. Nitrate in the city's water shows a very strong positive correlation with electrical conductivity (EC), sulfate, and total dissolved solids (TDS).

Wherever nitrate concentration is high, these three parameters will also be significantly elevated, and vice versa.

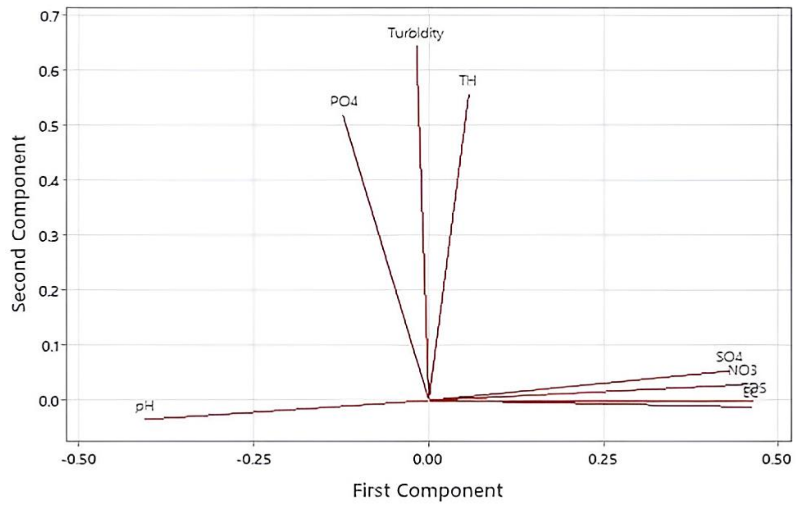

Fig. 5. The PCA loading plot

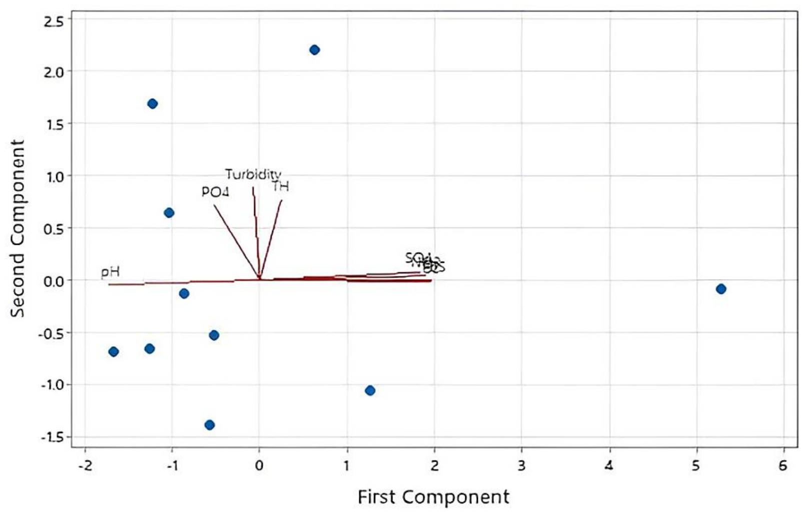

Fig. 6. The biplot of PCA

4. Conclusion

After sampling and measuring water parameters in accordance with Iran's national standards, the water quality index calculated for 8 variables and 10 water samples from Shahrekord's water distribution network, with an index value below 50, indicates that the drinking water quality in this city is excellent and very good. Following PCA conducted using Minitab22, it was determined that the first three components, covering a total of 84.8 % of the variance, are sufficient to represent the analysis process. The data are free of outliers. PC1, with the highest eigenvalue, is influenced by parameters such as sulfate, nitrate, electrical conductivity (EC), and TDS, indicating that salinity and chemical water quality are dominant. The second component, driven by phosphate, total hardness (TH), and turbidity, reflects the physical properties and hardness of water. The third component is associated with the contribution of phosphate and hardness. EC and TDS exhibit a high correlation.

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Author's contribution

Ahmad Shirani Takabi: Investigation, Methodology, data curation, Lab experiments, Conceptualization. Abolfazl Semnani and Saeed

Asadpour: Supervision and Editing the final draft, and. Mahboube Shirani: Validation, methodology, Advisor, Writing of original draft.

Conflict of interest

No potential conflict of interest was reported by the authors.

Data availability

The datasets generated and/or analyzed during the current study are available from the corresponding author on reasonable request.

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