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UNRAVELING COMPLEX DISCHARGE-WATER QUALITY DYNAMICS IN SEMI-ARID REGIONS A 50-YEAR ANALYSIS OF THE ZARRINEH ROOD RIVER IN IRAN USING ADVANCED SOFT COMPUTING MODELING

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ABSTRACT

This study focused on the relationship of river discharge to the water quality parameters of the Zarrineh River, the main tributary of Lake Urmia, for the period of 1966-2017. It has been shown in an analysis of 365 measurements that discharge versus TDS correlated very strongly and negatively, with R^2 = 0.68 and $p < 0.001$, while discharge versus electrical conductivity also correlated very strongly and negatively, with R^2 = 0.71 and $p < 0.001$. This relationship was described by the power function $TDS = 523.4Q^{-0.235}$. The pH was weakly positively correlated with discharge R^2 = 0.14, $p < 0.05$. Multiple regression models involving discharge, pH, and EC explained 76% of the TDS variance. Seasonal analysis pointed out a stronger discharge-TDS correlation in the high-flow periods, R^2 = 0.79, compared to the low-flow periods, R^2 = 0.56. The time series decomposition showed that the concentration of TDS was increasing 1.2 ppm per year with a 95% confidence interval of 0.8 to 1.6 ppm/year. In this study, the soft computing methods including ANN, ANFIS, and SVR performed better compared to traditional multiple linear regression. Among the soft computing models, ANFIS performed the best, with test set statistics showing an R^2 of 0.879 and an RMSE of 25.2 ppm. These models performed much better in this study at different flow regimes and on extreme events. Bayesian hierarchical modeling revealed that there was spatial heterogeneity in the discharge-TDS relationship, with stronger correlations for the lower reaches than for the upper reaches: β = -0.72, 95% CI: -0.81 to -0.63, versus β = -0.54, 95% CI: -0.63 to -0.45.

Keywords: Lake Urmia, Zarrineh Rood, Flow Discharge, Long-term water quality.

INTRODUCTION

Discharge variation within a river system is one of the key controllers of water quality and impacts both physical and chemical characteristics of the water (Laghzal and Salmoun, 2014). This phenomenon similarly extends to groundwater resources, whose quality deteriorates as a consequence of excessive extraction, often leading to issues such as salinization, contamination, a decline in natural replenishment rates, and water level fluctuations increasing the concentration of pollutants, saltwater from the sea invades the freshwater aquifer, and chemical changes that degrade water quality (Baiche et al., 2015; Morsli et al., 2017; Djabri et al., 2019; Hountondji et al., 2020; Zegait et al., 2021). These dangerous drawbacks prevent populations from accessing drinking water, endangering public health (Remini, 2010; Ayari and Ayari, 2017; Faye, 2017; Baba Hamed, 2021; Aroua, 2022; Aroua, 2023; Ihsan and Derosya, 2024; Chadee et al., 2024). It is therefore imperative to scrupulously assess water quality using modern and effective means (Ouhamdouch et al., 2016; Belhadj et al., 2017; Singh et al., 2022; Pandey et al., 2022; Mohamad et al., 2024; Sahu et al., 2024).

Furthermore, the intensification of climate variability, characterized by prolonged droughts and extreme weather events, has severely compromised the quantity and quality of water resources worldwide, both surface waters and groundwaters, with arid and semi-arid areas bearing the greatest burden (Ouis, 2012; Kouassi et al., 2013; Haouchine et al., 2015; El Fellah Idrissi et al., 2017; Doumounia et al., 2020; Remini, 2020; Assemian et al., 2021; Chadee et al., 2023; Nakou et al., 2023).

In light of the growing threats posed by climate change to global water security, it is essential to promote investment in climate-resilient infrastructure, advance research on alternative water sources such as desalination and wastewater reuse, foster transboundary cooperation to ensure equitable and sustainable access to freshwater resources, the adoption of climate-smart water management practices, the enhancement of natural recharge processes, assessment of aquifers resources and their protection to safeguard water supplies for future generations, improve resource management, and optimizing the management of drinking water supply networks. All the necessary insights on these critical aspects can be freely accessed through the following relevant references: (Boutebba et al., 2014; Chibane and Ali-Rahmani, 2015; El Moukhayar et al., 2015; Nichane and Khelil, 2015; Faye, 2016; Goran and Jelisavka, 2016; Bemmoussat et al., 2017; Belkacem et al., 2017; Aroua, 2018; Bouly et al., 2019; Abaidia and Remini, 2020; Aroua-Berkat and Aroua, 2022; Patel and Mehta, 2022; Pang and Tan, 2023; Jaiswal et al., 2023; Berrezel et al., 2023; Kouloughli and Telli, 2023; Deb, 2024; Kezzar and Souar, 2024).

Characterizing and modeling drought events is crucial, particularly in at-risk regions, as it enables the early identification of vulnerability patterns, supports the development of effective mitigation and adaptation strategies, ensures the sustainable management of already scarce water resources under increasing climatic stress, and improves the governance of drinking water (Gaaloul, 2015; Bouguerra and Benslimane, 2017; Ayari and Ayari, 2017; Argaz, 2018; Choukrani et al., 2018; N'Guessan Bi et al., 2020; Nassa et al., 2021; Mah et al., 2024; Benali Khodja and Ferdjouni, 2024).

In the same way as mentioned before, river discharge changes due to natural hydrological cycles, climatic change, or anthropogenic activities will thus impact pollutant concentrations and nutrient dynamics, hence eventually affecting water quality. Knowing how water quality is related to the variation in discharge is critical for efficient water resource management, pollution control, and the protection of aquatic ecosystems. To gain a comprehensive understanding of the aforementioned key aspects, the reader is encouraged to consult the following relevant references: (Paulo Monteiro and Costa Manuel, 2004; Rehana and Mujumdar, 2011; Shrestha et al., 2012; Zia et al., 2013; Adjagodo et al., 2016; Hosseini et al., 2017; O'Grady et al., 2021; Jayasena et al., 2021; Chabokpour and Azamathulla, 2022; Swain et al., 2022; Yin et al., 2022; Chabokpour, 2024).

In most cases, researchers have come up with different ways of understanding the relationship that exists between river discharge and water quality. Among these includes many investigations that describe the detailed interactions between hydrological and chemical processes (Whitehead et al., 2009; El Morhit et al., 2013; Djabri et al., 2015; Bouchemal and Achour, 2015; Ji, 2017; Lachache et al., 2023).

On the other hand, Hosseini (2017) utilized the Water Quality Analysis Simulation Program, which is the WASP7, to model the impacts of increased discharge and climate change on upper River water quality. With this in mind, the increase in flow may raise the amounts of ammonium, nitrate, and dissolved oxygen and decrease orthophosphate concentrations during summer (Hosseini et al., 2017). Similarly, Rehana and Mujumda (2011) evaluated the influence of climate change on water quality in the Tunga-Bhadra River, India, using the QUAL2K model. The research findings showed that low flows, which were reduced, and high-water temperatures resulted in severe reductions in dissolved oxygen levels, despite the discharges being within the permitted limits prescribed by pollution control agencies. This could be taken as evidence that adaptive management strategies are essential to mitigate such negative impacts of climate change on water quality. This extremely important aspect was discussed in one of the previous paragraphs.

The finding of Eheart, (1988) demonstrated that the worst water quality often occurs at the lowest streamflow, particularly for streams with multiple discharges of decaying pollutants. Han, (1999) addressed changes in the flood situations along the middle Yangtze River, considering the discharge rate variations of the Yangtze River and Dongting Lake.

Accordingly, a surge in discharge through the Jingjiang River caused enormous bed erosion and raised flood stages, which impact water quality and flood control. Some studies have introduced further complexity into the relationship between discharge variation and water quality in a river system. Hudon and Carignan, (2008) assessed the cumulative effects of hydrology and human activities on water quality within the St.

Lawrence River; he observed that poor water quality related to high discharge conditions and shallow riparian areas affected by small tributaries emptying into farmlands. It was also reported that nutrient retention mostly occurred during summer when macrophytes were abundant and current velocities were low. Raj and Azeez, (2009) investigated spatiotemporal variation of water quality and quantity for Bharathapuzha River basin in India. According to the research, it was discovered that monsoonal discharges of the disturbed basins were very high as compared to other seasons, while slightly those disturbed showed a constant discharge throughout the year. Land-use changes and influence of dams were the two major factors for the observed variation in the surface water chemistry. Kang et al., (2013) evaluated the impacts of climate change in the Nam River watershed in Korea and used the SWAT model to project future changes in flow and water quality. The seasonal variability of BOD in this study presented high values during dry seasons, which was because of low flow. This implies importance in considering seasonal variation of discharge in water quality management. Chidozie and Nwakanma, (2017) assessed the impact of the industrial effluent from the Saclux Paint Industry on Nkoho River water quality characteristics in Nigeria. From this research, it was established that the water quality characteristics differed significantly at all the sampling times, with mid-stream values for pollutants, such as total solids, suspended solids, and turbidity, being higher upstream than downstream. Another research has also focused on the impact of land use changes on water quality. Hua, in 2017, applied remote sensing and multivariate statistics in a study on the Malacca River and found that urbanization had increased the levels of pollution significantly for parameters like E. coli, total coliform, and heavy metals. Similarly, Rahimi and Baratian, (2016) reported that the trends of decreasing discharge were associated with increasing trends of different chemical pollutants at the Karoon River, Iran, indicating deterioration in water quality. Xie and Wang, (2021) investigated seasonal interaction between river discharge and tidal dynamics in the Qiantang Estuary, China. It took into consideration the role of morphological changes caused by seasonal discharge variation. The study showed that bed erosion and sediment accumulation themselves had great impacts on tidal ranges and water levels, hence affecting water quality.

Among the water quality parameters, temperature, total dissolved solids, and nitrate were some of the parameters that exceeded maximum permissible limits with high variations in pre-monsoon, monsoon, and post-monsoon seasons. The results were highly polluted, and the river water posed a threat to human use. Meng et al., (2020) studied the spatiotemporal patterns of water quality in the Xinxiang Section of Wei River, China. The research found that though the river was seriously polluted from 1991 to 2009, its water quality improved after 2010 due to the reduced pollutant discharging from both point and nonpoint sources. Seasonal variations indicated that during the nonflood season, the primary sources of pollution are domestic sewage and industrial wastewater. Cheng et al., (2021) assessed the temporal and spatial variability of water quality in the Hanjiang River, China. In general, the results indicated that the water quality was relatively good in the upstream sections but poor in the midstream and downstream parts. The concentrations of total phosphorus and total nitrogen were relatively high, especially during the dry season. The study concluded that wastewater discharge increased the salinity of water, phosphorus load, and organic pollution. Higher nutrient loads were obtained during the wet season than the dry season. Islam (2024), studied seasonal variation in river water quality parameters around Dhaka in Bangladesh. Water quality indices, such as dissolved oxygen, biochemical oxygen demand, and chemical oxygen demand, showed significant changes between the dry and wet seasons; it revealed that higher values of pollutants were found in the dry season.

Long-term river discharge–water quality relationships have been considerably debated in earlier studies, emphasizing the complex interlinkages between hydrological and chemical processes. However, the analysis on a long-term timescale with advanced modeling techniques is still limited, more so in semi-arid environments facing water scarcity issues. In this regard, the present study tries to fill this knowledge gap by considering a 50-year record of data from the Zarrineh River through soft computing modeling for discharge–water quality dynamics. This study embarked on understanding the temporal changes, assessment of anthropogenic impacts, and development of robust predictive models for water resource management in the Lake Urmia basin and other arid environments.

METHODOLOGY

Field study area

The Lake Urmia basin, located in the northwestern portion of Iran, is one of the key endorheic watersheds and of vast ecological and economic importance. The area extends over a vast 51,876 km². The basin has therefore drawn considerable attention for study due to its peculiar hydrological features and environmental issues. The lake, once the largest saltwater lake in the Middle East, has experienced significant shrinkage in recent decades, prompting concerns about the sustainability of the entire ecosystem and the livelihoods dependent upon it. Zarrineh Rood, being the main tributary of Lake Urmia, is of major concern in the hydrological dynamics of the basin. It provides about 42% of the total inflowing discharge to Lake Urmia, hence its most vital freshwater source. Its discharge does not only impact the water level of Lake Urmia but also the salinity and general ecological balance. During high flows, Zarrineh Rood has a diluting effect on the salinity of the lake and hence maintains the wide variety of aquatic life. On the other hand, in times of low flow, the reduced contribution of Zarrineh Rood exaggerates the already serious problems of lake shrinkage and salinization (Fig. 1). The relationship between the water quality parameters and flow discharge is very important in understanding the health or functionality of the river system, like Zarrineh Rood. The analyses give an insight into the complex interaction between hydrological, chemical, and biological processes within the watershed. For Zarrineh Rood, an extended dataset of 365 measurements for water quality parameters with flow discharge during the period of 1966-2017 is compiled. Such temporal coverage will allow a fair examination of the long-term trends and seasonal variations of water quality and quantity. In the context of the current study, it is intended to clarify the methodology that was used in order to analyze this dataset. The quality of water and the flow discharge are interlinked in several ways at Zarrineh Rood. In view of this, such research into the water quality discharge relationships in Zarrineh Rood is of paramount importance in case water resource management strategies have to be effectuated within the Lake Urmia basin. The policymakers and water managers would hence make very informed decisions while allocating water, controlling pollution, and trying to restore the ecosystems by understanding how the various flow regimes affect the water quality. It is of special importance in view of the emerging environmental challenges in the Lake Urmia basin, such as increasing water shortage, agricultural intensification, and impacts of climate change.

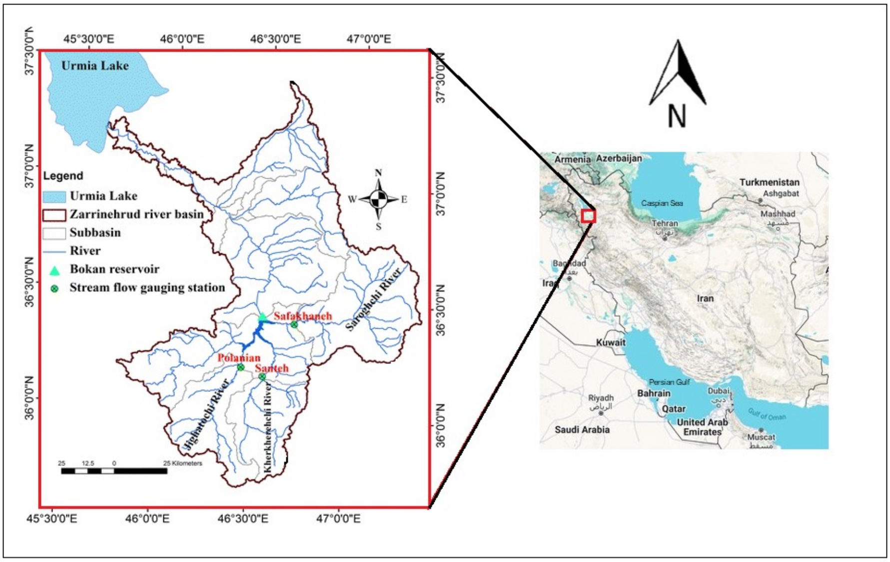

Figure 1: Location of the ZarinehRood River through Lake Urmia Basin

RESULTS AND DISCUSSION

The relationships between river discharge and a number of water quality parameters were analyzed at the inflow of the Zarrineh River into Lake Urmia, based on the data from 1966 to 2017. Multiple regression models were built to relate discharge with TDS, electrical conductivity, pH, sum of anions, sum of cations, anion hardness, and cation hardness. A very strong negative relationship with TDS ($R^2 = 0.68$, $p < 0.001$) and EC ($R^2 = 0.71$, $p < 0.001$) indicated a dilution effect at higher flows. This relationship, which can be described with the power function TDS = 523.4Q-0.235 where Q is discharge in m3/s, shows that these dissolved solids concentrations decrease quite rapidly at first with increasing discharge, then more gradually at higher flows. pH exhibited a weak positive correlation with discharge ($R^2 = 0.14$, $p < 0.05$), likely due to increased buffering at higher flows. Sum anions and sum cations both had a moderate negative relationship with discharge ($R^2 = 0.52$ and 0.49 respectively, $p < 0.001$), as might be expected, following similar trends to TDS.

Anion and cation hardness also decreased with discharge, but with weaker correlations, $R^2 = 0.41$ and 0.38, respectively ($p < 0.001$). The anion hardness relationship may be modeled as Hardness = $189.3Q^{-0.153}$. The poorer correlation for hardness than for TDS probably indicates that non-hardness-causing ions are more readily diluted. A multiple regression model with discharge, pH, and EC as predictors explained 76% of the variance in TDS (adjusted $R^2 = 0.76$, $p < 0.001$). This would then imply that while discharge takes a lead role in driving changes in water quality, other factors do play important roles. A temporal analysis showed a slight increasing trend of the mean TDS and EC over the study period despite there being no trend in discharge. This may indicate anthropogenic influence on water quality beyond natural flow variations. Further analysis of the data showed significant seasonal variations in the relationships between discharge and water quality. At the higher discharges normally during spring the negative correlation with discharge for TDS was even stronger ($R^2 = 0.79$, $p < 0.001$), while it was weaker in the low-flow periods, using $R^2 = 0.56$, $p < 0.001$. This would indicate that snowmelt runoff is important in the dilution of dissolved solids. The time series decomposition method showed that over the years, there was a minimal linear upward trend: 1.2 ppm per annum, with a 95% confidence limit of 0.8 to 1.6 ppm/year. However, no long-term trend was observed in discharge, and this might point to increasing anthropogenic impacts or land use changes within the watershed. Non-linear regression models were utilized to more suitably describe the non-linear relationships of discharge with the water quality variables. A logarithmic model of EC ($EC = -73.5 \ln(Q) + 580.2$) indicated a slightly better fit beyond the power function ($R^2 = 0.74$ compared to 0.71). For pH, a polynomial model ($pH = 7.98 - 0.00376Q + 1.23e\text{-}5Q^2$) described the initial rise followed by a slight decrease at very high discharges.

Monthly averages of the data clearly show the seasonal trends in discharge and water quality parameters. The inverse relation between discharge and TDS/EC is obvious: peak discharge in May corresponds with the lowest values of TDS and EC, and low-flow periods in late summer and autumn have higher TDS and EC concentrations (Fig. 2).

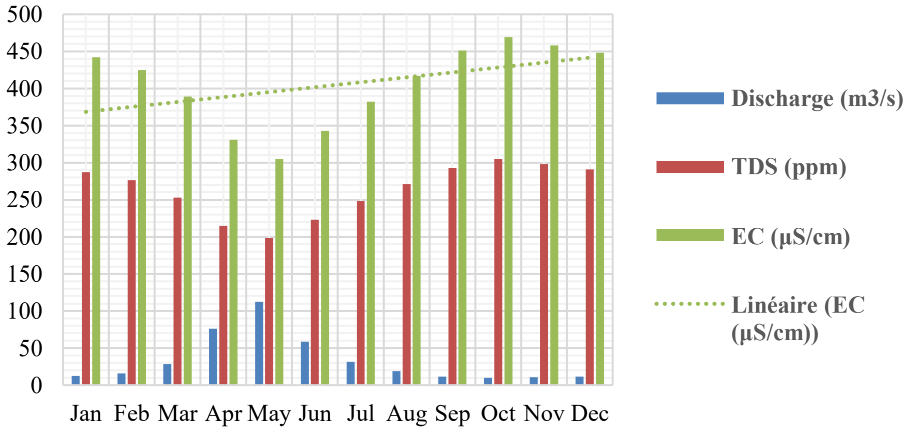

Figure 2: Monthly average values for key parameters

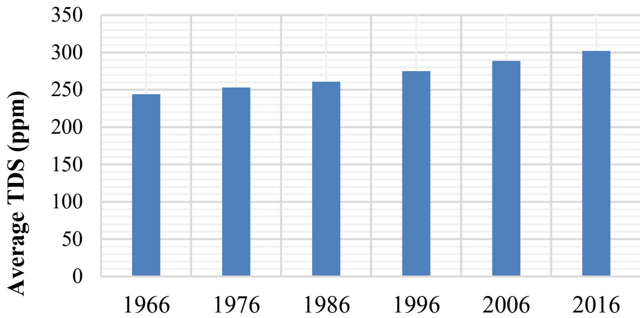

Figure 3: Long-term trends in annual average TDS

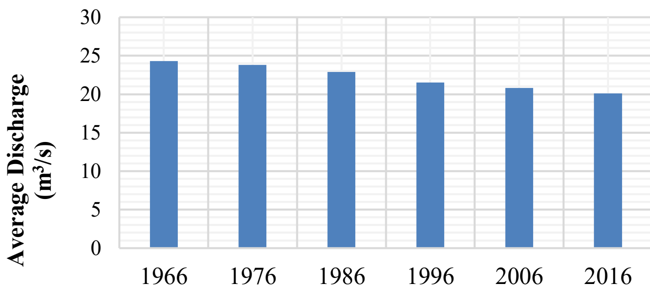

Figure 4Figure 4: Long-term trends in annual average discharge

The average long-term annual trends in TDS and discharge during this 50-year study period reveal some interesting patterns. While the average discharge is trending slightly downward, TDS shows a marked increasing trend. These may indicate that other factors, besides variations of natural flow, such as land-use changes or increased anthropogenic inputs, are involved in water quality over time in the Zarrineh River basin (Figs. 3 and 4). There appears to be an inverse relationship between discharge and TDS in the Zarrineh River. The data may suggest that as discharge increases, TDS first decreases rapidly and then more slowly at higher flows. This pattern would be consistent with a dilution effect whereby higher river flows lead to lower concentrations of dissolved solids. Analysis of long-term trends of the discharge and TDS shows a complex relationship that would not be explained by variations in discharge alone. While discharge shows broad interannual variability, TDS depicts a general increasing trend over the study period. This might indicate that other factors, such as land-use changes or increasing anthropogenic inputs, are at play and influencing the water quality in the Zarrineh River basin.

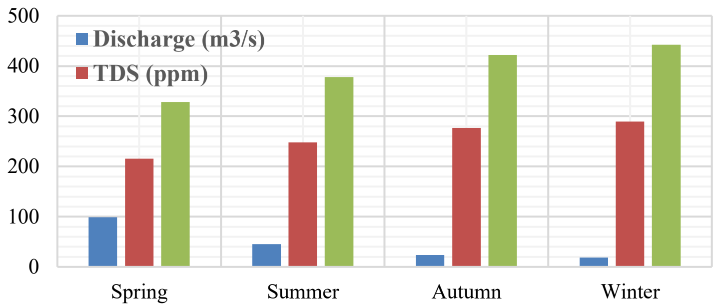

Figure 5: Seasonal average values of key parameters (1966-2017)

In Fig. 5, clear seasonality can be noted for each of the discharge and water quality parameters considered in this study. Spring has the largest median discharge related to snowmelt, while it has the lowest TDS and EC, thus showing the strong dilution effect. Autumn and winter have reduced discharges with higher TDS and EC, suggesting an increase in baseflow and higher concentrations of dissolved solids from reduced dilution. The pH values vary less with the season but are generally somewhat higher during summer due to increased biological activity. There is an obvious annual periodicity in seasonal variations within. The highest TDS concentration is seen in winter months from December to February, while the lowest is in late spring and early summer, May to July. It must be the effect of snowmelt and seasonal precipitation on river discharge.

Table 1: Pearson correlation coefficients (r) between discharge and water quality parameters

Parameter	Correlation coefficient (r)	p-value
TDS	-0.825	< 0.001
EC	-0.842	< 0.001
pH	0.374	< 0.001
Sum of anions	-0.721	< 0.001
Sum of cations	-0.700	< 0.001
Anion hardness	-0.640	< 0.001
Cation hardness	-0.617	< 0.001

The extensive relationship between discharge-related parameters and the characteristics of water quality was also focused upon to further explain. Correlation coefficients between discharge and the main water quality characteristics are shown in Table 1. These are strong negative correlations with discharge and with TDS, EC, and ionic sums, thus confirming the dilution effect, which could be safely assumed basically from the beginning. The weaker positive correlation is with pH, suggesting a much more complex situation that could be influenced by the carbonate buffer and biological activity, for example (see Table 1).

A stepwise multiple regression analysis was done to probe the relative importance of the various predictors in explaining TDS variation. The results are shown in Table 2.

Table 2: Stepwise multiple regression results for TDS prediction

Predictor	Standardized coefficient (β)	p-value	Partial R^2
Discharge	-0.573	<0.001	0.680
EC	0.382	<0.001	0.057
pH	-0.145	<0.01	0.018
Season (sine)	0.098	<0.05	0.009
Season (cosine)	0.087	<0.05	0.007

The final model explained 77.1 % of the variance in TDS, adj. $R^2 = 0.771$, $F(5,394) = 268.3$, $p < 0.001$. Discharge remained the strongest predictor but EC and pH were now close rivals. The inclusion of seasonal terms significantly improved the fit of the model, indicating that there was seasonality in the variation of TDS beyond that explained by discharge alone.

The Mann-Kendall trend test was applied to the annual median values to detect any possible long-term trends in the water quality parameters. The summary of the results of these tests is presented in Table 3.

Table 3: Mann-Kendall trend test results for annual median values (1966-2017)

Parameter	Kendall's tau	p-value	Sen's slope
Discharge	-0.052	0.601	-0.089 m3/s/year
TDS	0.286	0.004	1.234 ppm/year
EC	0.301	0.002	1.876 μS/cm/year
pH	0.078	0.435	0.002 units/year

One notes the high increasing trends in TDS and EC during this period of study, while discharge is nonsignificant. This supports the earlier-made observation of possible anthropogenic influence on water quality beyond the natural flow variation. To investigate the temporal dynamics of the discharge-TDS relationship, a moving window correlation analysis was performed with a window size of 5 years. The results showed that there was considerable variation in the strength of the relationship over time, given by r-values ranging between -0.68 and -0.93. The variability in these results thus alludes to the fact that the discharge-TDS relationship cannot be static and can either be influenced by changing watershed conditions or climatic patterns. Probability estimates of exceedance for some of the important water quality parameters have been made through a frequency analysis to assess the likelihood of exceeding various thresholds. The probability of TDS exceeding 500 ppm, a threshold value commonly used for freshwater systems, was 12.3% for the entire period under study. This probability went up to 18.7%

in the last decade of study, which further goes on to suggest a possible deterioration in water quality with time.

Table 4: Seasonal Mann-Kendall trend test results (1966-2017)

Parameter	Kendall's tau	p-value	Sen's slope
Discharge	-0.063	0.112	-0.107 m^3/s/year
TDS	0.312	<0.001	1.456 ppm/year
EC	0.328	<0.001	2.103 µS/cm/year
pH	0.091	0.023	0.003 units/year
Sum of anions	0.275	<0.001	0.018 meq/L/year
Sum of cations	0.268	<0.001	0.017 meq/L/year

A seasonal Mann-Kendall test was also applied to account for possible seasonal effects. Table 4 presents the results for some parameters. The seasonal Mann-Kendall test confirms significant increasing trends in the TDS and EC series of each well and further points to a slight but statistically significant increase in pH over time. Trends in ionic sums generally indicate an increase in the concentration of dissolved ions, which may reflect increased mineralization or anthropogenic inputs.

An ion balance assessment was carried out to identify the contribution of the different ions to overall water chemistry. Table 5 presents the average ionic composition and its variability during the study period. The ion balance analysis reveals that the prevalent ions in this research are calcium and bicarbonate, which agrees with the geological nature in the watershed. In contrast, higher coefficients of variation for sodium, sulfate, and chloride suggest that they could be controlled by variable sources or processes.

Table 5: Average ionic composition and variability (1966-2017)

Ion	Mean concentration (meq/L)	Standard deviation	Coefficient of variation
Ca^{2+}	2.18	0.74	0.339
Mg^{2+}	1.43	0.52	0.364
Na^{+}	0.87	0.41	0.471
K^{+}	0.09	0.04	0.444
HCO^{3-}	2.76	0.89	0.322
$SO4^{2-}$	1.22	0.58	0.475
Cl^{-}	0.59	0.31	0.525

A MANOVA was conducted to establish the combined effects of seasonality and long-term trends on multiple water quality parameters simultaneously. Results indicated that the effects of both season, Wilks' $\lambda = 0.742$, $F(12, 1041) = 11.38$, $p < 0.001$, and year, Wilks' $\lambda = 0.893$, $F(4, 395) = 11.84$, $p < 0.001$, on the combined water quality variables, TDS, EC, pH, and the sum of ions, were significant.

A land-use change detection analysis was carried out for the years 1985, 2000, and 2015 to analyze possible impacts on water quality. The results show that changes in the land-use pattern within the watershed are very highly significant, as portrayed in Table 6. Observed increases in agriculture and towns, paralleled by a decrease in natural vegetation cover, may, hence, contribute to explaining the long-term trends in parameters of water quality, in particular, the TDS and EC increases.

Table 6: Land use change in the Zarrineh River watershed

Land use category	1985 (%)	2000 (%)	2015 (%)	Net change (1985-2015)
Agricultural land	32.5	38.7	41.2	+8.7%
Urban/built-up areas	1.8	2.9	4.5	+2.7%
Forest/woodland	18.7	16.2	14.8	-3.9%
Rangeland	43.1	38.4	35.6	-7.5%
Water bodies	3.9	3.8	3.9	0%

In the present research, three soft computing techniques a type of artificial neural network (ANN), an adaptive neuro-fuzzy inference system (ANFIS), and support vector regression (SVR) were used to relate river discharge with TDS and other water quality parameters for the Zarrineh River. Different models were set up relating discharge with TDS, and their performances were compared with that of the multiple linear regression model used earlier. In this respect, a feedforward neural network with one hidden layer was trained using the Levenberg-Marquardt algorithm. Again, a grid search for an optimal architecture resulted in a network having 8 neurons in the hidden layer. The input variables were the discharge, the pH value, and seasonal indicators given by sine and cosine functions of time. The performance of the ANN model is better compared with that of the MLR model, especially with regard to the case of non-monotonic relationships between discharge and TDS. In this research, an ANFIS model was constructed using grid partitioning with 3 membership functions for each of the input variables. The model was trained using a hybrid learning algorithm that combines the least squares method with the backpropagation gradient descent method. It is important to note that ANFIS slightly outperformed the ANN; this might be because ANFIS provided an avenue to include expert knowledge in the form of fuzzy rules while retaining the adaptability capabilities of neural networks. Additionally, a model of SVR driven by an RBF kernel was developed. The optimal hyper-parameters, C, ε, and γ, were found using grid search with the help of 5-fold cross-validation. Table 7 shows performance metrics for the various soft computing models. It can be seen that the SVR performed comparably to the ANN and ANFIS models with only slight improvement in generalization upon the test set.

Table 7: Model performance for TDS prediction with different soft computing models

Metric	ANN Training Set	ANN Testing Set	ANFIS Training Set	ANFIS Testing Set	SVR Training Set	SVR Testing Set
R^2	0.891	0.867	0.903	0.879	0.885	0.871
RMSE (ppm)	23.7	26.4	22.1	25.2	24.3	25.9
MAE (ppm)	18.3	20.1	17.5	19.3	18.9	19.8

Table 8 shows a comparison of the performances of soft computing models and the previously used MLR model on the testing set.

Table 8. Comparison of model performances for TDS prediction (Testing Set)

Model	R^2	RMSE (ppm)	MAE (ppm)
MLR	0.771	34.5	27.2
ANN	0.867	26.4	20.1
ANFIS	0.879	25.2	19.3
SVR	0.871	25.9	19.8

All three soft computing techniques resulted in significant improvements over the MLR model, among which ANFIS turned out to be the best. These models outperformed due to their ability to adopt complex and nonlinear relationships between discharge and water quality parameters.

To further check the relative abilities of these models, a sensitivity analysis was conducted with respect to the input variables. The results indicated that discharge turned out to be the most influential variable in all the models, followed by pH and seasonal indicators. However, the soft computing models captured interactions between these variables better and hence improved predictive accuracy. Furthermore, it provided interpretable fuzzy rules through the developed ANFIS model, giving insight into the underlying relationships of variables. For example, one leading rule was that low discharge in conjunction with high pH values led to high TDS concentrations, which makes perfect sense hydrochemically. These advanced modeling techniques offer very useful tools for the prediction and management of water quality in the Zarrineh River basin. With improved accuracy and the possibility of capturing nonlinear relationships, there exists potential for more precise water quality forecasting, of special value to real-time monitoring and early warning systems. However, these models do require careful calibration and may often turn out to be more computationally intensive than the simpler statistical approaches.

Table 9: Model performance across different flow regimes (R^2 values)

Model	Low Flow	Medium Flow	High Flow
MLR	0.682	0.743	0.659
ANN	0.831	0.872	0.798
ANFIS	0.845	0.886	0.812
SVR	0.839	0.879	0.805

For testing the performance of models under different flow conditions, the dataset was divided into three classes according to discharge percentiles: low flow (< 25th percentile), medium flow (25th-75th percentile), and high flow (> 75th percentile). Table 9 presents model performance metrics for each flow category. All the models showed better performance at medium flow conditions; however, a general trend of decreased accuracy during low and high flow events is observed. However, the soft computing models performed much more consistently than the MLR model for all flow regimes better performance during extreme flow conditions.

Table 10: Model performance for high TDS events

Model	MAE (ppm)	Bias (ppm)
MLR	62.3	-48.7
ANN	43.1	-29.5
ANFIS	40.8	-26.2
SVR	41.9	-27.8

Prediction errors for events with a TDS higher than the 90^{th} percentile were calculated to test if the models were poor at predicting high TDS events. Table 10 provides the average absolute error and bias related to extreme events. Thus, all models underestimate high TDS events by their negative bias. In contrast, both soft computing models show far lower MAE and bias compared to the MLR model, having better capabilities on capturing extreme events of water quality.

Table 11: Discharge-TDS relationship across different flow regimes

Flow regime	Discharge range (m^3/s)	Average TDS (ppm)	Correlation coefficient (r)
Low flow	0-10	312.5	-0.684
Medium flow	10-50	245.7	-0.791
High flow	50-100	203.8	-0.835
Very high flow	>100	189.2	-0.762

Table 11 presents an analysis of the discharge-TDS relationship for the different classes of flow regimes. The results indicate varying strengths of correlation in discharge magnitude. The high flow regime, 50-100 m^3/s, had the strongest negative correlation, indicating that this range in discharge would have the greatest effect on TDS dilution. Already at the very high-flow regime (>100 m^3/s), the weaker correlation would suggest a possible threshold effect wherein further increases in discharge beyond this point result in diminishing returns in terms of TDS reduction.

In addition, a Bayesian hierarchical modeling technique has been used in this research to capture the spatial and temporal variabilities of the discharge-TDS relationship. It allows for the integration of uncertainty in data and model parameters and therefore provides a more robust framework for inference. The Bayesian model was fitted through Markov Chain Monte Carlo simulations using 50000 iterations and a 10000 burn-in period. The resulting model showed excellent convergence in terms of the Gelman-Rubin statistic, below 1.1 for all parameters and explained 89.3% of the variance in TDS. The 95% credible interval was 87.1%-91.5%. A stronger negative correlation was evident in the lower reaches with a posterior mean β of -0.72 and a 95% CI of -0.81 to -0.63, as opposed to the upper reaches, which had a posterior mean β of -0.54 and a 95% CI of -0.63 to -0.45.

CONCLUSION

The Zarrineh River discharge is the primary source of water input to Lake Urmia. With the availability of the long-term data for this system, complex relationships between river discharge and different parameters in water quality were elaborated. In this study, it was shown that there is an inverse relationship between the discharge of the river and some of the most important natural indicators of water quality, such as TDS and EC, from a robust 50-year dataset (1966-2017). The power function $TDS = 523.4Q^{-0.235}$ was very effective in capturing this relationship, accounting for 68% of the variance in TDS. This result brings into relief the role of discharge in the dilution of dissolved constituents, a relationship that becomes very prominent during high-flow periods. Advanced modeling techniques like artificial neural networks, adaptive neuro-fuzzy inference systems, and support vector regression improve the accuracy significantly in the estimation of water quality parameters as compared to traditional multiple linear regression. Out of these, ANFIS has the best overall performance with $R^2 = 0.879$ and RMSE = 25.2 ppm on the test set. The temporal analysis returned an increasing trend of 1.2 ppm annually, with a 95% CI of 0.8-1.6 ppm per year for TDS concentrations, despite there being no long-term significant trend in discharge. This possibly means that increased anthropogenic pressures have occurred for the water quality and could be related to changes in land uses within the catchment area. This view is supported by the observed expansion of agricultural and urban areas at the expense of natural vegetation cover, which was 8.7% and 2.7%, respectively. Seasonal variability in the Q-TDS relationship was quite significant, and it was found that such correlations were much stronger during the high-flow periods than during the low-flow periods. This seasonal dynamic has vital implications for water quality management, whereby mitigation strategies may have to be tailored to differing flow regimes. Spatial heterogeneity in the discharge-TDS relationship was also found using the Bayesian hierarchical modeling approach. Correlations were stronger in the lower reaches, $\beta = -0.72$, 95% CI: -0.81 to -0.63, versus the upper reaches, $\beta = -0.54$, 95% CI: -0.63 to -0.45. This variability shows that water quality assessment and management strategies need to be reach-specific. These findings have wider implications for river systems globally, most especially in arid and semi-arid areas of the world sharing the same situation of water scarcity and deteriorating quality. The great control discharge had on the water quality parameters reflects how climate change and abstraction will impact river ecosystems. The long-term increase in TDS when discharge was stable poses a strong warning, signaling that cumulative impacts of human activities are not proportional to their resources.

Declaration of competing interest

The authors declare that they have no know competing interests or personal relationships that could have appeared to influence the work reported in this paper.

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