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Groundwater Quality Analysis by Integrating Water Quality Index, GIS Techniques and Supervised Machine Learning: A Case Study in Duhok Province, Iraq

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ABSTRACT

This paper presents a case study, focusing on the analysis of the Water Quality Index (WQI) using ArcGIS Pro and supervised machine learning (SML) techniques. The study aims to analyze the selection of physicochemical water quality indicators in water wells to determine the most effective physicochemical water quality parameters in water wells, in addition of finding WQI of each well at Duhok province and its purpose of use. These parameters include Calcium, Magnesium, Chloride, Sodium, Potassium, Sulfate, pH, Electrical Conductivity (EC), Total Dissolved Solids (TDS), Nitrate, Total Alkalinity (TA), and Total Hardness (TH).

The study generated a spatial distribution map of the WQI, revealing the highest values in wells located in the Sumil district, ranging between 18.47-57.9, while the lowest value of 18.47 was observed in the Akre district. Supervised machine learning algorithms were employed to identify the most influential physicochemical indicators on water quality. The results highlighted EC, TA, TH, and Ca+2 as the most crucial parameters affecting WQI. The mapping analysis further indicated that wells in the Sumil district exhibited the highest values of EC, TH, Mg+2, and TA Conversely, the Duhok district demonstrated the highest calcium levels, while the lowest pH and nitrate levels were observed in the Duhok and Amedi districts, respectively. The Zakho district showcased the highest levels of sulfate and potassium, and the Bardarash district had the highest chloride and sodium values.

KEYWORDS: Water Quality Index; Groundwater Quality; Supervised Machine Learning; Geographic Information System (G.I.S.); Water Resources Management.

1 INTRODUCTION

Water wells have been an essential element in the development of human societies throughout history, providing a reliable and consistent source of clean water for residents (Misstear, Banks and Clark, 2007). One of the oldest well discoveries is in Cyprus, dating from 7000 to 9000 BC (Fagan, 2011). Wells continue to have an essential role in society today since more than 3 billion people worldwide likely rely on water wells for their drinking water supplied directly from drilled or hand-dug wells (World Health Organization and Fund (UNICEF), 2014). The condition of a well can deteriorate over time due to various factors such as industrialization, contamination from human activities, and ageing infrastructure. Therefore, monitoring a well's water quality is essential to ensure that the water is safe and suitable for its intended (drinking, irrigation, industrial or commercial) uses and to prevent any negative impacts on human health, the environment, and the economy. Regular monitoring can address any issues in water quality early to identify the sources of contamination and perform any necessary repairs or maintenance to ensure its continued functionality prior to making any threats. Overall, monitoring the quality of groundwater is a critical aspect of managing and protecting our water resources, ensuring that they remain safe, sustainable, and available for future generations (World Health Organization, 2011; World Health Organization, 2012).

There is a growing need for effective techniques for a healthy life that allow for better interpretation of water quality data. These techniques include using water quality indices (WQIs), which provide an optimized numerical value to represent the overall water quality of a sample (Naubi et al., 2016; Chidiac et al., 2023; Lumb, Halliwell and Sharma, 2006; Şener, Şener and Davraz, 2017). A Water Quality Index (WQI) is a composite indicator that considers several parameters that affect water quality, including physical, chemical, and biological characteristics. The index is calculated based on the measured values of various parameters, such as pH, temperature, dissolved oxygen, turbidity, and other chemical constituents. Each parameter is assigned a weight based on its importance to water quality, and the overall index is then calculated by combining the weighted scores of all the parameters using the weighted arithmetic index method (Adelagun et al., 2021). Different ranges of WQI values may correspond to different categories of water quality, such as excellent, good, fair, poor, or very poor. This information can be used to make informed decisions about water resource use, treatment, and management (World Health Organization, 2004).

In addition, Supervised Machine Learning (SML) such as Decision Tree Forest and Tree Boost can be used to analyze and interpret large datasets of water quality measurements. These techniques involve using algorithms to train models on historical data, allowing them to make predictions or classifications on new data and identifying the most critical factors influencing the water quality index in a particular location (Su et al., 2021; Ma et al., 2020; Khaledian et al., 2018; Kazi et al., 2009). Decision trees create a tree-like structure of decisions based on the input features. The model starts with a root node representing the entire dataset and splits it into smaller subsets based on the input features. Each split is based on a condition that maximizes the information gain or minimizes the impurity in the subsets. The final leaves of the tree represent the most effective physicochemical parameters on WQI for all subsets (Khoi et al., 2022).

Into the bargain, to make spatial related research more valuable and informative, it is crucial to use G.I.S. data to better visualize any specific geographical area (Nazif, 2019). So that ArcGIS is a powerful G.I.S. software that can be used for a wide range of geospatial analysis tasks, including spatial interpolation techniques like Kriging. Kriging is a statistical method for estimating the value of a variable at a specific location based on the values of neighboring points (Alcaras et al., 2022). Several research studies have highlighted the importance of using G.I.S. data to generate kriging models to analyze water quality index (WQI) parameters. For instance, a study by (Al-Waeli et al., 2021) used G.I.S. data to generate a kriging model for WQI parameters in Baghdad city and found that the resulting maps effectively identified areas with high and low water quality. Similarly, a study by (Masood et al., 2021) used G.I.S. and Kriging to generate spatial models of WQI parameters in Mewat district, state of Haryana in India, to understand better drinking water quality.

The key aim of this study is to find the most effective physicochemical water parameters of Duhok province, Kurdistan Region of Iraq, by integrated WQI data and supervised machine learning, besides utilizing ArcGIS Pro powered by G.I.S. data to run a spatial interpolation technique called Ordinary Kriging. Thus Kriging maps offer several benefits for visualizing and analyzing spatial data.

2 CASE STUDY

This case study determined and analyzed the water quality index (WQI) of 189 wells in Duhok Province, Kurdistan Region, Iraq. The study aimed to analyze these wells' most effective physicochemical water quality indicators using ArcGIS Pro and supervised machine learning techniques.

The study covered the seven districts of Duhok Province, namely Akre, Bardarash, Amedi, Shikhan, Duhok, Simul, and Zakho, as shown in Figure 1. Water samples were collected from each district and analyzed for various physicochemical parameters such as pH, electrical conductivity (EC), total dissolved solids (TDS), total alkalinity (TA), total hardness (TH), calcium (Ca^{+2}), magnesium (Mg^{+2}), potassium (K^{+}). chloride (Cl^{-}), sodium (Na^{+}), sulfate (SO_4^{-}) and nitrate (NO_3^{-}).

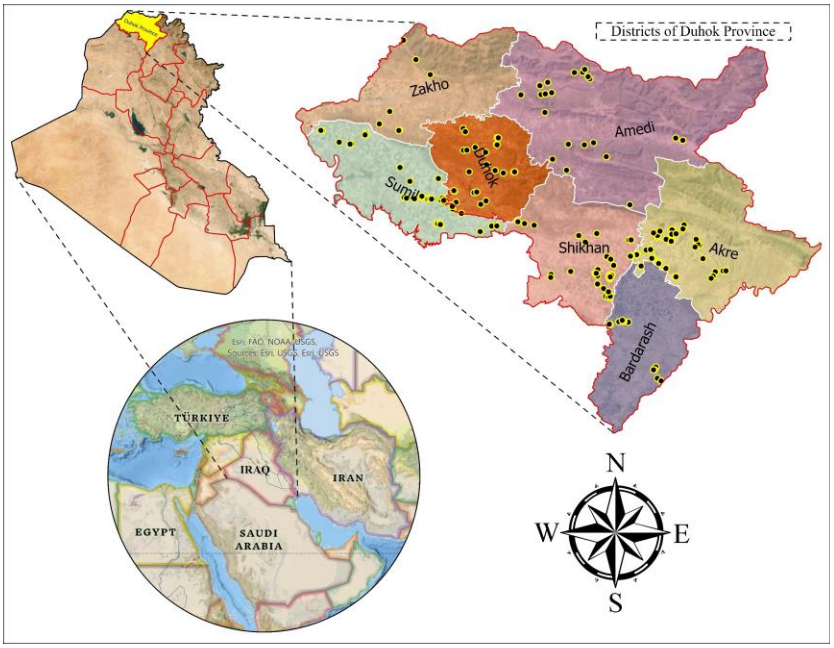

Figure 1: Case Study Area and Wells Distribution Point in Duhok Province Districts

3 METHODOLOGY

The Duhok Environmental Directorate, conducted a meticulous assessment of 189 water well samples in Duhok Province, following the guidelines set by the World Health Organization (WHO), to find 12 essential water physicochemical parameters. The author then calculated Water Quality Indices (WQIs.) using the Weighted Arithmetic Index Method, as detailed in **Table 4**. The evaluations were necessary to determine the quality of the water and ensure that it met the required standards for human consumption and other uses.

3.1 Water Quality Index (Weighted Arithmetic Index Method)

The weighted arithmetic index method is commonly used for calculating the water quality index (WQI). Overall, Water Quality Index (WQI) is based on several parameters that affect the overall quality of water. Among the parameters used to calculate WQI, some are considered ionic groups, some are physical, and others are chemical.

The ionic groups include calcium (Ca+2), magnesium (Mg+2), chloride (Cl-), sodium (Na+), potassium (K+), and sulfate (SO4-). These ions can affect water's taste, odour, and suitability for various uses.

The physical parameters include pH, electrical conductivity (EC), and total dissolved solids (TDS). pH measures the acidity or basicity of water, while EC measures the electrical conductivity of water, which is related to the presence of dissolved salts. TDS measures the total amount of dissolved water substances, including ionic and non-ionic.

The chemical parameters include nitrate (NO3-), total alkalinity (TA), and total hardness (TH). Nitrate levels can significantly impact the health of aquatic ecosystems and human health, while T. A. is related to the chemical composition of water. TH measures the amount of calcium and magnesium ions in water, which can cause scale buildup in pipes and appliances (A. Melloul and Collin, 1992).

Therefore, understanding the different types of parameters that affect water quality and their impact is crucial for assessing the suitability of water for various uses and ensuring its safe and optimal utilization.

The process of calculating the WQI involves the following steps (World Health Organization, 2011):

A- The first step is to calculate the sub index or quality rating (qn) for each water quality parameter. If there are n parameters, the qn value reflects the relative value of these parameters in the polluted water compared to the standard permissible value. The following formula is used to calculate qn:

qn = 100($[Vn - V0]/[Sn - V0]$) ………………. (1)

Where **qn** is the quality rating for the **nth** parameter, **Vn** is the observed value of the nth parameter at a given sampling station, **Sn** is the standard permissible value of the nth parameter as shown in **Table 1**, and **Vo** is the ideal value of the nth parameter in pure water. For all parameters except pH whose ideal value is 7.0, the ideal values are set to zero for drinking water (Tripathy and Sahu, 2017).

Table 1: Recommended WHO Standards for drinking water quality (World Health Organization, 2004).

Parame-ters	PH	EC (µs/cm)	TDS (mg/l)	No3- (mg/l)	TA (mg/l)	TH (mg/l)	Ca+2 (mg/l)	Mg+2 (mg/l)	Cl- (mg/l)	Na+ (mg/l)	K+ (mg/l)	So4- (mg/l)
Stand-ards	8.5	400	1000	50	200	300	75	50	250	200	12	250

B- The second step is calculating each water quality parameter's unit weight (Wn), which is inversely related to the standard value Sn. The formula for calculating Wn is:

Wn = K/Sn ……………………(3)

Where **Wn** is the unit weight for the nth parameter, **Sn** is the standard value for the nth parameter, and **K** is a constant of proportionality (K=1/(Σ1/Sn).

C- Finally, the WQI is calculated using the following formula:

WQI = $\Sigma qnWn/\Sigma Wn$………………………. (4)

The WQI is determined as shown in **Table 4** as an example of WQI calculations.

Then WQI value is classified into five categories. **Table 2** shows the five water quality classifications based on the WQI technique of the weighted arithmetic index method.

Table 2: Water quality classification based on WQI value for drinking proposes (Tiwari et al., 2009)

No.	**WQI level**	**Water quality classification**	**Purpose of uses**
1	0-25	Excellent	Drinking and irrigation
2	26-50	Good	Drinking and irrigation (Slightly Polluted)
3	51-75	Poor	Irrigation and treatment are needed before drinking
4	76-100	Very poor	Need attention for irrigation
5	More than 100	Unfit and unsuitable for drinking	Unfit for all uses

3.2 Supervised Machine Learning

Supervised machine learning algorithm was used to identify the most effective physicochemical water quality indicators for predicting WQI in the wells by implementing Tree Boost technique.

Tree Boost is an ensemble learning algorithm that creates a sequence of decision trees, with each subsequent tree built to correct the errors of the previous tree. The algorithm was trained as shown in **Table 3** using 12 water quality data of 189 wells, as mentioned previously to identify the most important water quality parameters affecting WQI. Furthermore, for the assessment of the ultimate performance outcomes of the supervised machine learning (SML) model, a collection of previously unseen data was examined as a test against the trained data to validate its performance.

Table 3: Tree Boost model settings

Tree Boost Parameters	**Value**
Max. Number of Trees in Series	500
Depth of Individual Trees	7
Min. Size Node to Split	10

The proportion of Rows for Each Tree	0.5
Huber's Quantile Cutoff	0.95
Influence Trimming Factor	0.01
Shrink Factor	Auto
Surrogate Variables	**Value**
Number of Surrogates to Store	5
Minimum Surrogates Association	60
General	**Value**
Fitness Function	R^2
Number of data rows	189
Target	WQI
Variables	12 Parameters

3.3 Ordinary Kriging

Ordinary Kriging was used in ArcGIS Pro to generate kriging maps that visualize the spatial distribution of each water quality parameter. Kriging is a geostatistical interpolation method that predicts the values of unknown points based on their spatial relationship with known points.

To generate Kriging maps, the water quality data was imported into ArcGIS Pro, and the spatial coordinates of the wells were used to create a point layer. The layer was then interpolated using Ordinary Kriging to generate a continuous surface of each water quality parameter.

The kriging maps were used to identify areas with high and low water quality and detect any spatial patterns or trends in the data. The maps were also utilized to validate the results of the supervised machine learning algorithms by comparing the predicted values with the actual values of each water quality parameter at different locations.

4 RESULTS AND DISCUSSION

As outlined in Methodology Section 3.1, the formulas and steps for computing WQI are described. **Table 4** present calculations to illustrate this process.

Table 4: An instance of calculating the water quality index for one well among the 189 wells.

Parameters	Observed values (Vn)	Ideal Value (Vo)	BIS Stand-ards(Sn)	1/Sn	Unit weight (Wn)	Quality In-dex (qn)	qn.Wn
PH	7.3	7	8.5	0.117	0.421	20	8.429
EC (µs/cm)	507	0	400	0.0025	0.009	126.765	1.135
TDS (mg/l)	325	0	1000	0.001	0.004	32.452	0.116
No3- (mg/l)	8.04	0	50	0.02	0.072	16.089	1.153
TA (mg/l)	196	0	200	0.005	0.018	98	1.755
T.H (mg/l)	316.00	0	300	0.0033	0.012	105.333	1.258
Ca+2 (mg/l)	78.40	0	75	0.0133	0.048	104.533	4.993
Mg+2 (mg/l)	29.28	0	50	0.02	0.072	58.56	4.196
Cl- (mg/l)	16.00	0	250	0.004	0.014	6.4	0.092
Na+ (mg/l)	6.90	0	200	0.005	0.018	3.45	0.062
K+ (mg/l)	1.20	0	12	0.083	0.299	10	2.985
So4- (mg/l)	76.59	0	250	0.004	0.014	30.635	0.439
∑				**0.1781**	**1**		**26.613**

WQI = $\Sigma qnWn / \Sigma Wn$ = 54.379 / 1 = **26.613**

The study results indicated that the WQI values of the water wells in Duhok Province varied widely, ranging from 18.47 to 57.9. In comparison to the ranges provided by the World Health Organization (WHO) in **Table 2**, the WQI values of approximately 18% of the wells were categorized as poor, 10% as Excellent and 70% good (Slightly polluted) as shown in **Figure 2**.

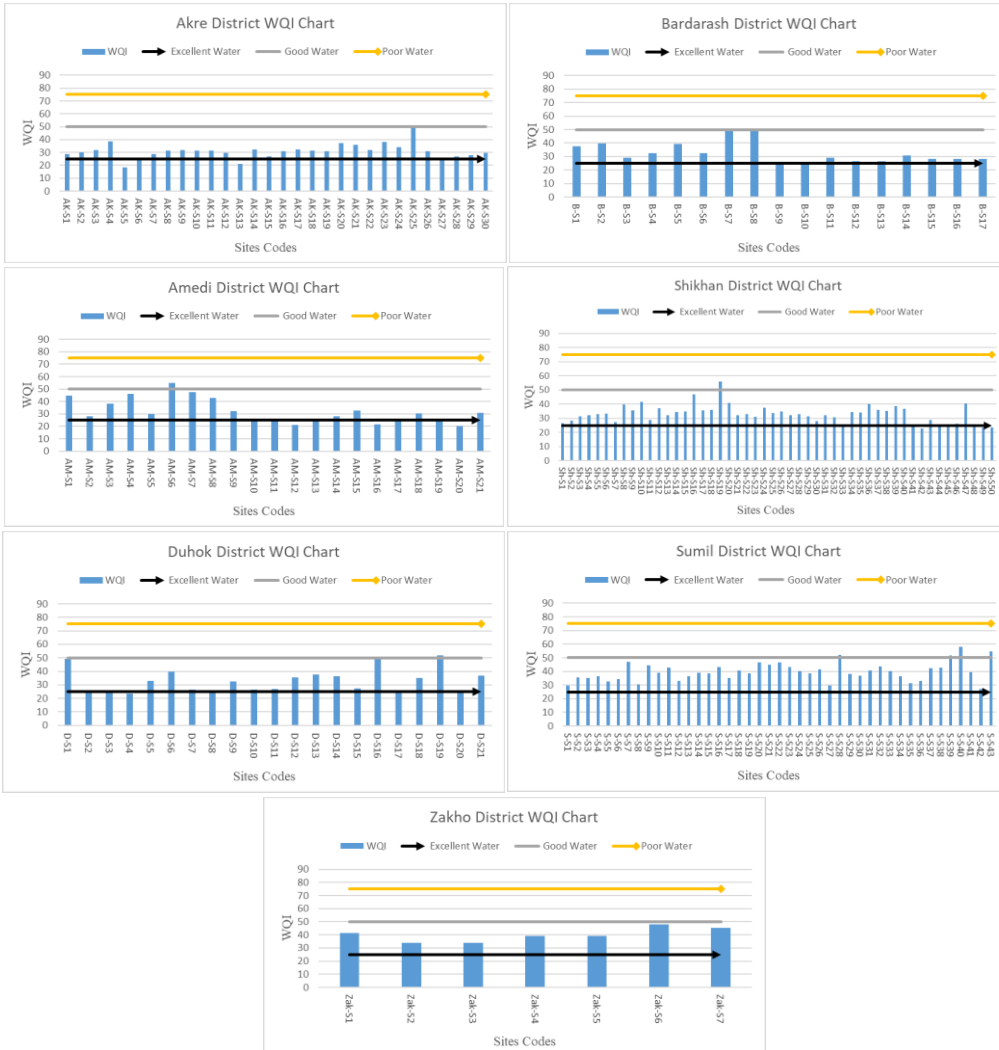

Figure 2: Water Quality Indices of all districts of Duhok province wells

Obtaining drinkable water requires meticulous control and precise evaluation of various parameter groups related to water quality and comparing the water quality parameters to WHO standards provides a benchmark for assessing the suitability of the water for human consumption. Ionic groups, encompassing calcium, magnesium, chloride, sodium, potassium, and sulfate ions, significantly influence water quality. These ions can affect taste, odor, and the overall suitability of water for drinking. Therefore, closely monitoring and managing the concentrations of these ionic groups is essential to ensure the water is safe and enjoyable to consume, obviously as shown in **Figure 3** the concentration of calcium, magnesium, and sulfate in the majority of wells at Duhok province appears to exceed the standards set by the World Health Organization (WHO). As a result, these elevated levels have an impact on the overall water quality.

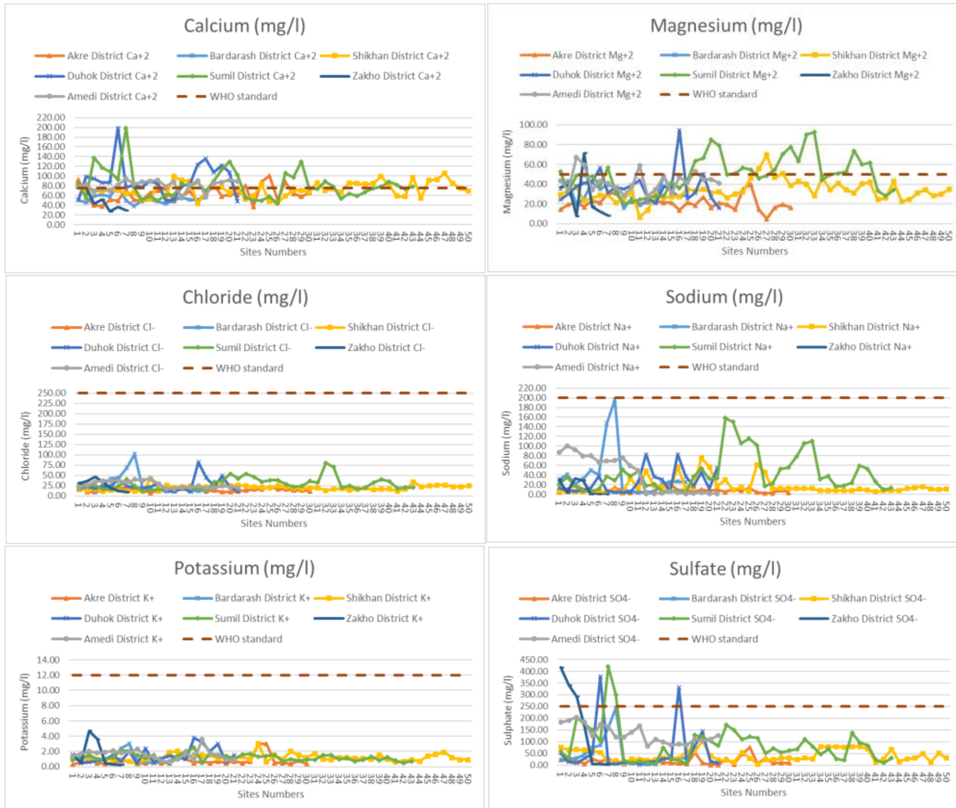

Figure 3: Ionic groups of water quality parameters at Duhok province

Also, physical parameters, such as pH, electrical conductivity (EC), and total dissolved solids (TDS), provide valuable insights into water characteristics. pH levels indicate the acidity or alkalinity of water, which impacts taste and its compatibility with the human body. Monitoring electrical conductivity and TDS helps assess the presence of dissolved substances. Controlling these physical parameters ensures that the water meets the necessary standards for drinkability. However, in Duhok province, it is crucial to have dissolved substances present in the water wells because the electrical conductivity (EC) ratio is significantly higher than the standards set by the World Health Organization (WHO) as shown in **Figure 4.**

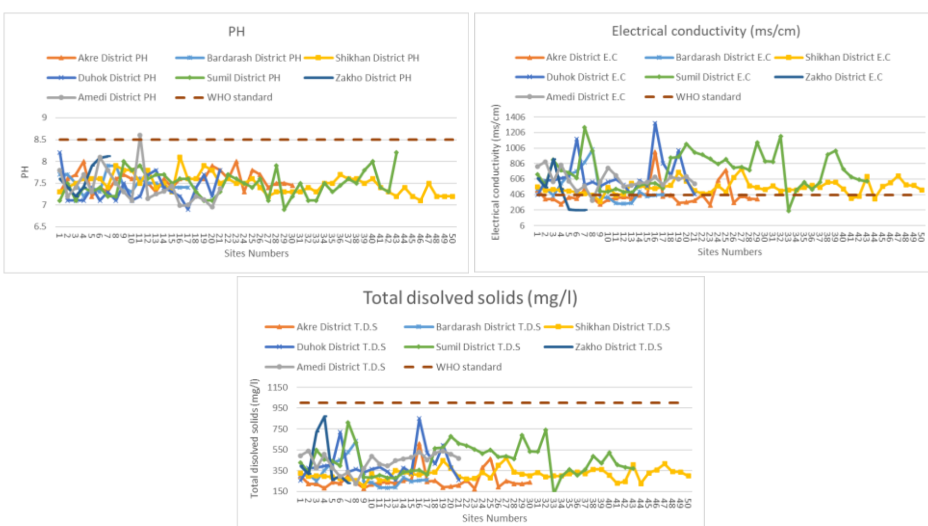

Figure 4: physical parameters of water quality at Duhok province

Furthermore, chemical parameters, including nitrate, total alkalinity (TA), and total hardness (TH), require careful attention. Elevated nitrate levels in water, often originating from agricultural or industrial sources, can pose health risks. Total alkalinity indicates water's ability to resist changes in pH, while total hardness refers to the presence of calcium and magnesium ions, affecting taste and causing scaling issues. So that the high concentration of chemical parameters in the water wells across all districts of Duhok province leads to an increase in water quality issues, resulting in poor drinking water conditions, as shown in **Figure 5**. However, maintaining appropriate levels of these chemical parameters is crucial for obtaining water that is safe and suitable for consumption.

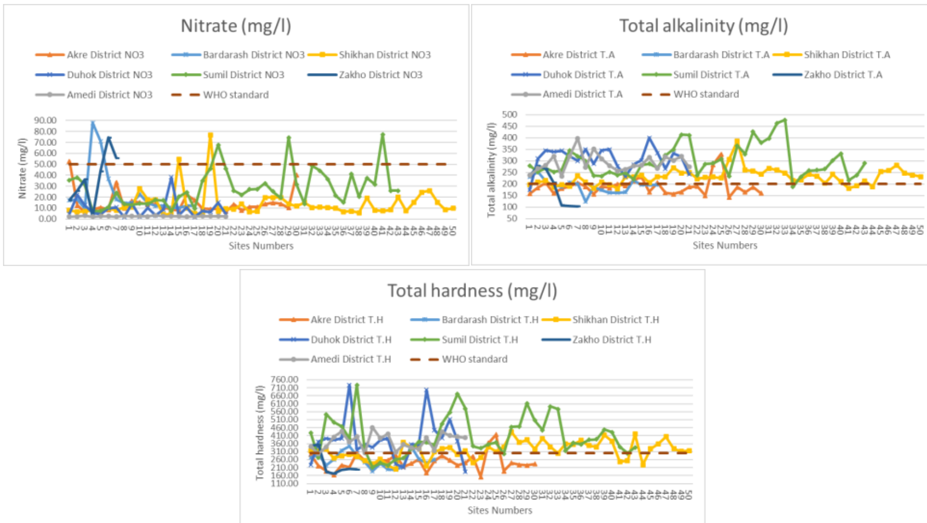

Figure 5: chemical parameters of water quality at Duhok province

By effectively monitoring and controlling (ionic groups, physical and chemical parameters) water treatment facilities, regulatory bodies, and individuals can take necessary actions to eliminate contaminants, and ensure overall water quality.

To make it obvious, supervised machine learning algorithms were used to identify the most effective physicochemical water quality indicators on the WQI of the wells. The results showed that the most prominent parameters affecting WQI were Electrical Conductivity (EC), Total Alkalinity (TA), Total Hardness (TH) and Calcium (Ca+2), for both trained and tested data.

The Tree Boost algorithm achieved a proportion of variance (R^2) equal to 94.097% in predicting the importance of variables as shown in the **Table 5** for case study database at Duhok Province.

Table 5: Overall Importance of Variables on WQI for Tree Boost algorithm at Duhok Province

Variables	Importance
EC	100%
TA	92.741%
TH	60.689%
Ca+2	38.300%
No3-	19.447%
Mg+2	9.911%
So4-	8.803%
PH	3.665%
Na+	2.449%
Cl-	1.362%
K+	0.853%
TDS	0.398%

The kriging maps generated using ArcGIS Pro provided a visual representation of the spatial distribution of each water quality parameter. The Ionic groups map as shown in **Figure 6**, indicated that the districts of Sumil, Duhok, and Amedi have the highest concentrations of calcium (Ca+2) and magnesium (Mg+2). Additionally, the Amedi district exhibits widespread high levels of chloride (Cl-), sodium (Na+), potassium (K+), and sulfate (SO4-). Additionally, the Akre district is primarily characterized by the lowest concentrations of ionic groups.

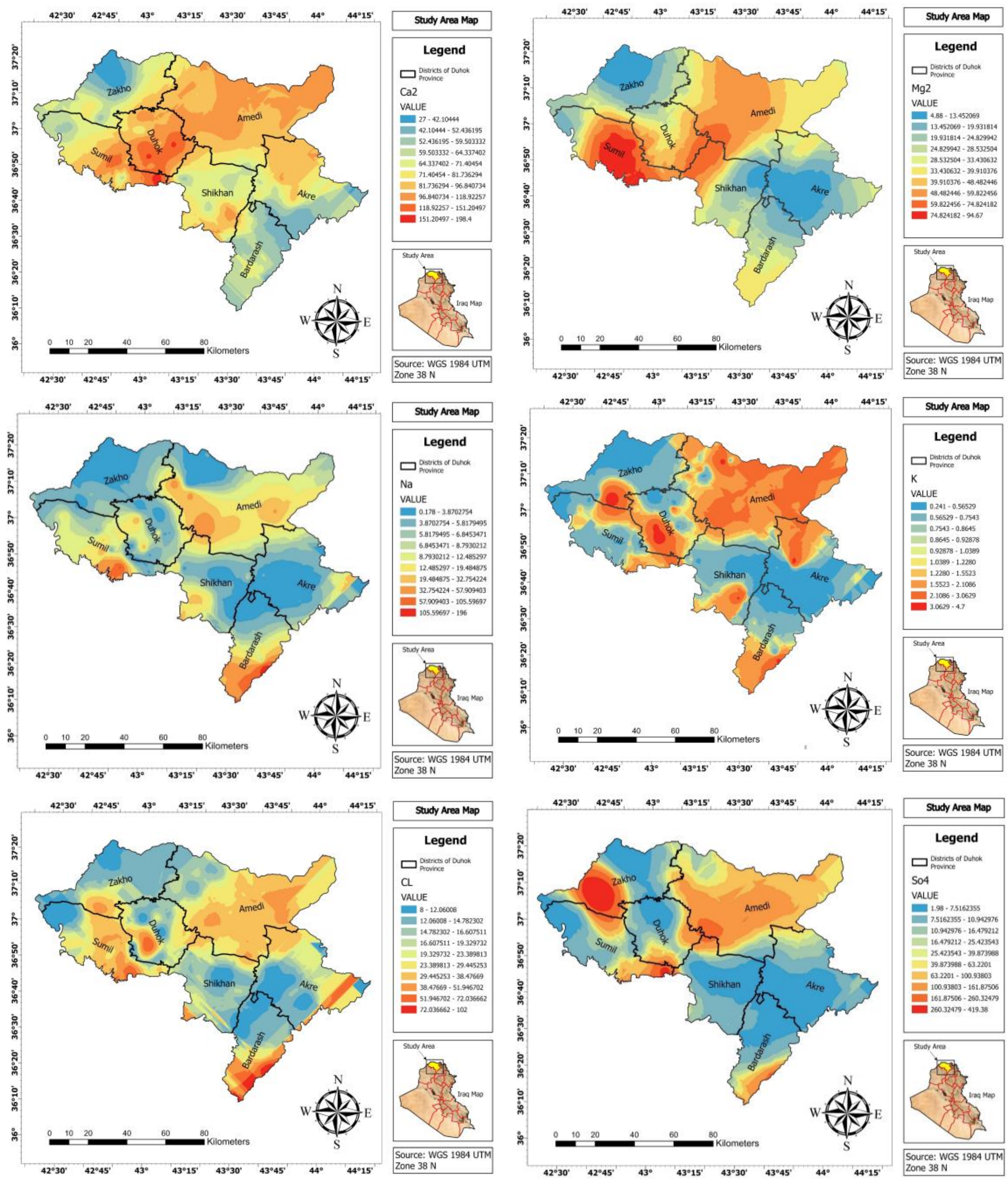

Figure 6 : Spatial Distribution of Ionic groups

On the other hand, Physical parameters map as shown in **Figure 7**, revealed that pH has the highest rate at Zakho district and the lowest value around Amedi district. Over and above that electrical conductivity (EC) and total dissolved solids (TDS) have the highest rates at Sumil districts and the lowest rates at Akre districts.

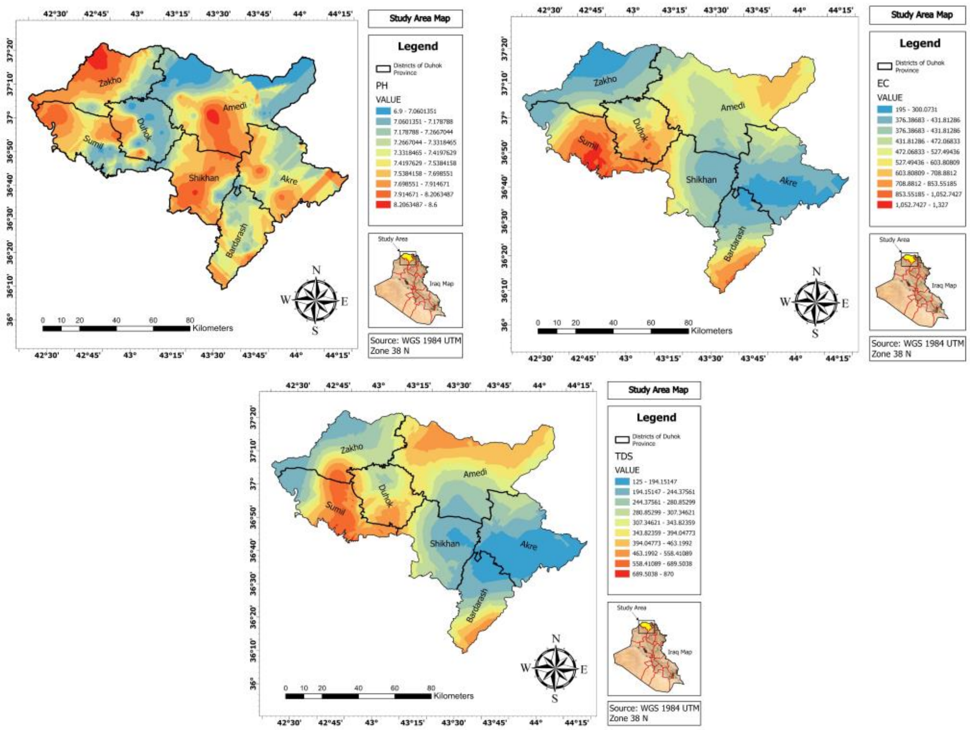

Figure 7 : Spatial Distribution of Physical parameters

Figure 8, which depicts the Chemical parameters map, reveals that Zakho district has the highest concentration of nitrate (NO3-) while Amedi district has the lowest. Moreover, Sumil district exhibits the highest levels of total alkalinity (TA) and total hardness (TH), whereas Akre district records the lowest levels of both.

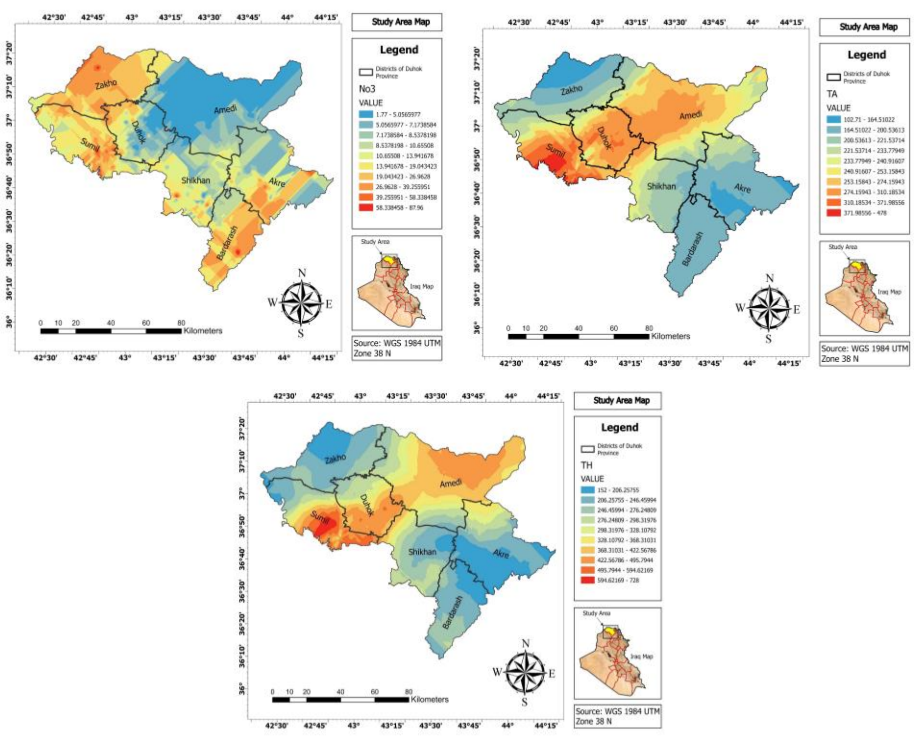

Figure 8 : Spatial Distribution of Chemical parameters

In **Figure 9**, the Kriging spatial distribution map of WQI illustrates that the wells in Sumil district have the highest value, while the lowest value is observed in the Akre district.

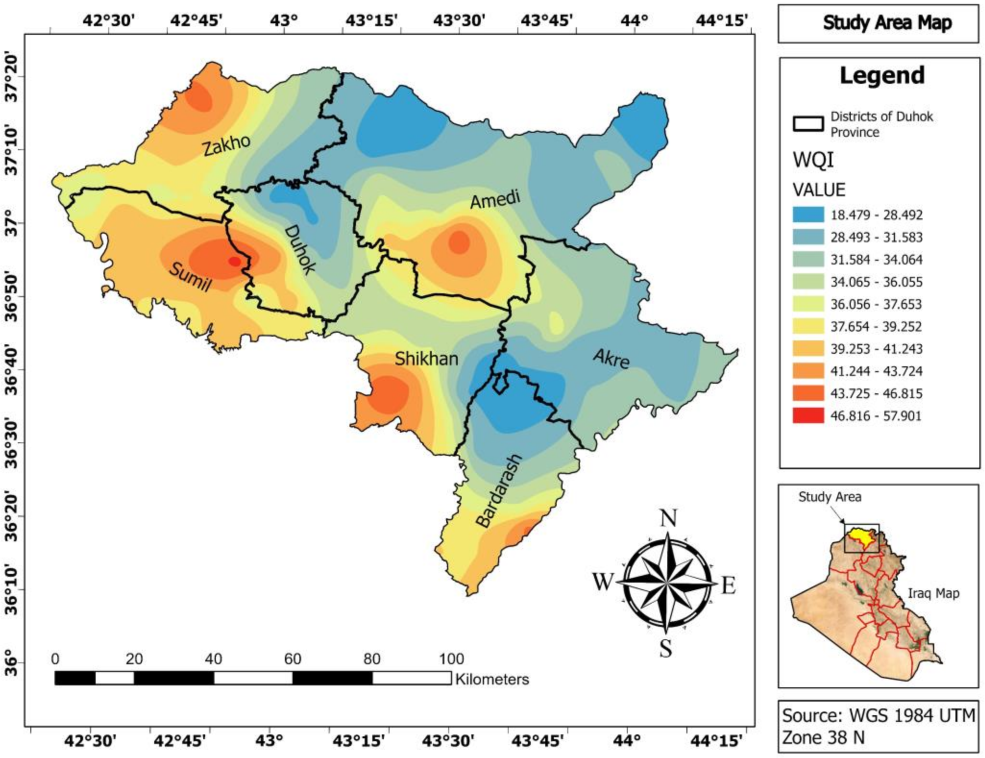

Figure 9 : Spatial Distribution of WQI in Duhok province

5 CONCLUSION

In conclusion, the analysis using supervised machine learning has identified four key parameters - Electrical Conductivity (EC), Total Alkalinity (TA), Total Hardness (TH) and Calcium (Ca+2) - that significantly influence the water quality index (WQI). Additionally, it's worth noting that the values of Electrical Conductivity (EC), Total Alkalinity (TA), Total Hardness (TH), and Calcium (Ca+2) parameters exceed the range defined by the WHO Standard as shown in the **Figures 4, 5 and 6**. The Kriging spatial distribution maps further reveal that these parameters have the highest levels in the Sumil district. Combining the results from both analyses (Kriging spatial distribution maps and supervised machine learning) , it can be concluded that the Sumil district has the highest WQI values because these four parameters are the most effective indicators of physicochemical water quality, as determined by supervised machine learning. As a result, the Sumil district's WQI is the highest due to the strong impact of these parameters. These findings are crucial for policymakers and water resource managers, emphasizing the need for targeted interventions to improve water quality in the Sumil district. By addressing these influential factors, we can protect human health, preserve ecosystems, and ensure sustainable use of water resources for future generations.

Overall, the study's results demonstrate the significance of integrating G.I.S. data, supervised machine learning, and geostatistical techniques with water quality parameters for analyzing ground water quality. The approach can help identify the most effective water quality indicators and provide valuable information for managing and improving water resources in the study area.

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