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Spatial statistical analysis of groundwater quality based on inverse distance weighting and ordinary kriging in District Sheikhupura, Pakistan

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ABSTRACT

Groundwater is an important source of fresh drinking water in Pakistan and it has a great impact on human and ecological health. Therefore, it is imperative to evaluate the quality of groundwater. This study aims to explore the spatial variability of groundwater quality and to predict the unmeasured locations in Sheikhupura, Pakistan. For this purpose, hydro-chemical results of 105 water samples were taken from the Pakistan Council of Research in Water Resources (PCRWR). The water quality parameters including total dissolved solids, calcium (Ca), magnesium (Mg), hardness, sodium (Na) and sulfate (SO_4) were measured from each sample at every location and compared with the permissible limits of the World Health Organization (WHO). Initially, descriptive statistical measures along with normality tests are carried out to assess the shape of water quality parameters. Later on, two geostatistical prediction techniques: inverse distance weighting (IDW) and ordinary kriging (OK) were considered to predict the unmeasured locations within the study domain. In this case, the parameters of the experimental variogram (sill, range and nugget) were estimated using the best-fitted variogram models including exponential, spherical, matern and Gaussian. Cross-validation statistics were carried out to evaluate the performance of IDW and OK. Results showed that the OK better performed than IDW. Furthermore, the water quality index was plotted to demonstrate the overall quality of groundwater in District Sheikhupura. It was observed that the area (South-West) with latitude 31.55°–31.66° and longitude 73.79°–73.93° have a very poor quality of groundwater. On the whole, only 9.6% of locations have excellent water for drinking. Thus results showed that the quality of groundwater is not satisfactory in Sheikhupura, Pakistan; therefore, serious preventive measures are required to reduce possible threats to human and ecological health.

Keywords: Groundwater; Health effects; Geographic information system; Water quality index; Sheikhupura

1. Introduction

Water is essential for the survival and development of life on Earth. Groundwater is an important source of fresh water and has a vital role to sustain agricultural, industrial and human activities [1]. Rapid growth in population, industrialization and urbanization has increased groundwater pollution [2]. Pakistan has sufficient surface and groundwater resources [3]. Most of the clean groundwater and drainage systems have parallel resemblances in the country. So, the groundwater is being contaminated due to leakage and melding [4]. Industries are also the main source of water pollution because industrial discharge is found to be hazardous for humans as well as the environment [5]. Around 92% of sewage water is directly discharged into rivers and groundwater [6]. In Pakistan, the level of groundwater is falling a meter per year due to the extraction for agricultural and drinking purposes [7]. According to the World Bank

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report, only 36% of people in Pakistan have access to safe and clean groundwater [8].

Sheikhupura, being an industrial estate play a vital role in the economy of Pakistan. Major industries of this area include textile, leather, rice, steel, paper, pharmaceutical and poultry. Most of these industries discharge their wastage into rivers and groundwater [9]. Consequently, the problem of water contamination arises, leading to a harmful impact on humans and the environment [9]. The quality of groundwater is assessed by the presence of eminent levels of toxic chemicals and their health effects [10]. The US Environmental Protection Agency (EPA) has inspected that groundwater contains more than 200 organic compounds [6]. The important physiochemical contaminants that cause severe health diseases are electric conductivity (EC), power of hydrogen (pH), bicarbonate, calcium (Ca), magnesium (Mg), hardness, sodium (Na), potassium, sulfate (SO_4), total dissolved solids (TDS) and arsenic [11]. Groundwater with high levels of TDS causes gastric and bone diseases [12]. Contamination of sulfate in groundwater causes diarrhea and dehydration [13]. Whereas the excess quantity of magnesium and sulfate (>250) can have a laxative effect [14]. A hazardous level of pH may cause eyes and skin infections. Arsenic beyond permissible limits is also found to be a cause of skin, bladder and lung cancer [15].

The geostatistical analysis is quite popular for the assessment of physiochemical parameters of groundwater. Moreover, spatial techniques give optimal results to explore the problem under study. Geographic information systems (GIS), correlation and kriging have been found very useful techniques for water quality management [16]. Ishaku et al. [17] observed the groundwater quality by using GIS mapping and inverse distance weighting (IDW) interpolation technique in the Jada area of Northern Nigeria. They used ordinary kriging to estimate the spatial pattern of groundwater quality parameters (chloride, pH, sulfate, sodium, calcium, magnesium and hardness) in Ardabil, Iran [18]. Madhav et al. [19] evaluated that the quality of groundwater was deteriorated due to the anthropogenic and agricultural activities in the Kadawa River Basin, India. Kadam et al. [20] evaluated the quality of groundwater of 68 water samples by using multivariate statistical techniques. In another study, Ahmed and Ali [21] evaluated the impact of chemical processes and urbanization on groundwater quality in Sohag, Egypt. Cartographic maps were generated by using the multivariate statistical tools and IDW for thirteen physiochemical parameters in Dhamar, Yemen [22]. Hui et al. [23] evaluated the groundwater quality in Lianhuashan district, China, by using the water quality index and multivariate statistical techniques. Abbas and Cheema [24] assessed that the groundwater quality was not satisfactory and arsenic contaminant adversely affects human health in Sheikhupura, Pakistan. Maghami et al. [25] evaluated the groundwater quality of 27 wells using different interpolation methods (kriging, IDW and spline) in Abadeh. Several studies have been conducted to predict water quality parameters by using different interpolation techniques in Pakistan [26–31]. A water quality index (WQI) is a very useful tool to understand the general water quality status [32].

This study aims to predict the groundwater quality in Sheikhupura, Pakistan and its suitability for drinking purposes. For this purpose, 105 water samples were taken and analyzed for groundwater quality. The main objective of the study is, to identify the spatial extent of groundwater quality in Sheikhupura and to identify the significant association between the groundwater quality parameters by using geostatistical techniques. In the end, the overall groundwater quality of the study area was assessed through the WQI.

2. Methodology

2.1. Study area and data description

The study area of the present research is District Sheikhupura which is a well-known industrial city in Punjab, Pakistan. It became a district in 1919 with a total area of 3,030 km^2 and lies between 73°37'E to 74°41'E and 31°20'N to 33°05'N on the globe. It shares its boundaries with Lahore (South East), Gujranwala (North), Hafizabad (North), Narowal (North East) and Nankana Sahib (West) and in the east, the international boundary with Amritsar, India. According to the census-2017, its population was 3,460,426. The district has a severe climate from April to October summer season with temperature ranges from 30°C to 45°C and winter from November to March. Dust storm occurs during the June, July & August and the average rainfall during the year is about 635 mm [33]. Sheikhupura plays a vital role in Pakistan's economy and this industrial estate was established in 1969 with large-scale industries including (textile, leather, rice, steel, paper, pharmaceutical, poultry, etc.). These heavy industries make the water contaminated and their pollutants are extremely destructive for humans and the environment [9]. So there is a need to highlights, analyze and suggest some remedial measures in those areas where the water is contaminated for drinking purposes. For this purpose, a survey was conducted by the Pakistan Council of Research in Water Resources (PCRWR) in 2016 to assess groundwater quality. Fig. 1 shows the location map of the selected 105 samples of groundwater quality parameters from the District Sheikhupura, Pakistan. Groundwater samples were collected from the hand pumps, wells, taps, streams and water supply schemes. Clean sterile plastic bottles were used for groundwater samples and boric acid and nitric acid were used as preventive for trace elements. Samples were kept cool and dark while transporting them to the laboratory for chemical analysis. More detail of the chemical analysis of groundwater samples was given in the supplementary material section. Groundwater samples were examined for six physicochemical parameters which are more affect groundwater quality including total dissolved solids (TDS), calcium (Ca), magnesium (Mg), hardness, sodium (Na) and sulfate (SO_4). R-language and ArcGIS 10.7 software was used for the descriptive and geostatistical analysis of the measured water quality parameters.

2.2. Multivariate statistics

Multivariate statistical techniques are used to examine the relationship and significance between multiple groundwater quality parameters [34]. The coefficient of correlation, r_{ij} between ith and jth variables is defined as:

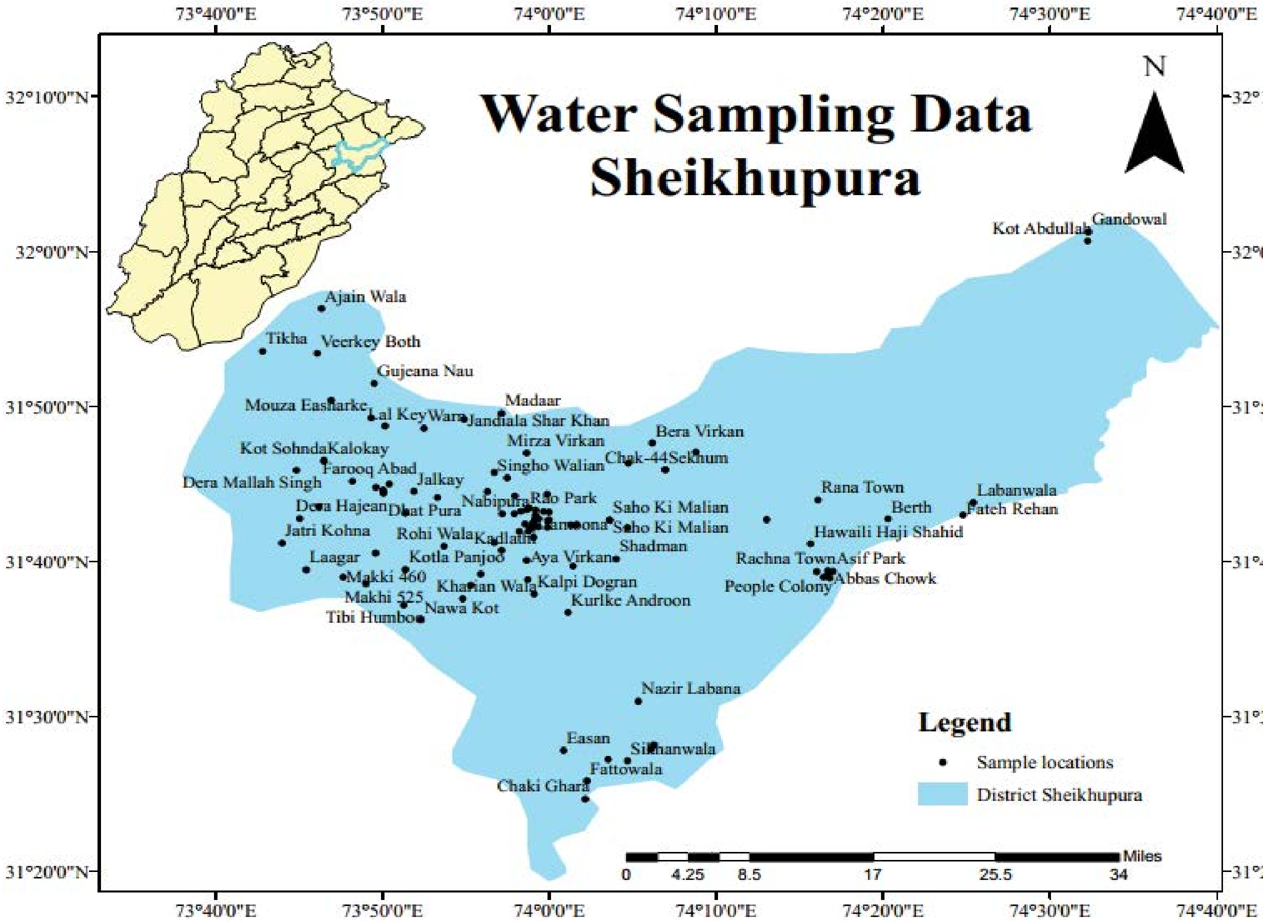

Fig. 1. Groundwater sample locations map of District Sheikhupura.

$$r_{ij} = \frac{s_{ij}}{s_i s_j} \quad i, j = 1, 2, 3, \ldots, t \tag{1}$$

where s_{ij} is the covariance between the ith and jth variables s_i and s_j are the standard deviations of ith and jth variables respectively. The correlation matrix D is extensively used to identify the most correlated parameters and is described as follows:

$$D = \begin{bmatrix} 1 & r_{12} & \cdots & r_{1t} \\ \vdots & \vdots & \ddots & \vdots \\ r_{t1} & r_{t2} & \cdots & 1 \end{bmatrix} \tag{2}$$

where t represents the number of variables and the values given as diagonal are the correlations of a variable with itself.

2.3. Data normalization

The first step in interpolation techniques is data normalization. In the present study, the Shapiro–Wilk [35] normality test was applied to check the normality of groundwater quality parameters (Table 1). To normalize the non-normal parameters, the Box–Cox [36] transformation was used as:

$$Y' = \begin{cases} \dfrac{Y^{\lambda} - 1}{\lambda} & \lambda \neq 0 \\ \log(Y) & \lambda = 0 \end{cases} \tag{3}$$

where Y' is the transformed variable and λ is the transformation parameter.

2.4. Variogram models

Before interpolating the un-gauged locations, it is quite important to assess the spatial correlation between neighboring sites. Semivariogram $\gamma(h)$ is used to detect the spatial dependence of the different neighboring locations [37] and described as:

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} \left[Z(x_i + h) - Z(x_i) \right]^2 \tag{4}$$

where $N(h)$ denotes the number of pairs separated by range h and h be the spatial distance among locations. $Z(x_i)$ is the observed measure at ungauged location x_i.

Semivariogram parameters are necessarily required for spatial prediction so the values of these parameters were

Table 1
Descriptive statistics of water quality parameters of Sheikhupura, Pakistan

Parameters	Minimum	Maximum	Mean	SD	Skewness	Shapiro test	*P*-value
TDS	134	2,094	722.83	400.21	1.59	0.86	0.0001
Calcium	22	108	56.45	20.48	0.80	0.94	0.0001
Magnesium	3.8	94.8	31.40	16.49	0.96	0.94	0.0002
Hardness	78	600	269.74	99.50	0.63	0.97	0.0104
Sodium	3	612	154.63	123.53	1.87	0.82	0.0001
Sulfate	14	490	127.60	97.87	1.89	0.80	0.0001

Note: *P*-value less than 0.05 is considered significant.

estimated by using well-known estimation techniques with the assistance of variogram models. Matern spatial covariance model is utilized to evaluate spatial covariance structure [38].

$$\gamma(h) = \tau^2 + \sigma^2\left(1 - \frac{|h|}{\theta}\right)^v k_v\left(\frac{|h|}{\theta}\right) \tag{5}$$

where k_v is the Bassel function of order v and (τ^2, σ^2, υ, θ and $|h|$) ≥ 0. Where τ^2, σ^2 and θ are the sill, nugget and range.

The exponential model for spatial correlation [38] is defined as:

$$\gamma(h) = \tau^2 + \sigma^2\left\{1 - \exp\left(\frac{|h|}{\theta}\right)\right\} \tag{6}$$

The mathematical equation for the exponential variogram model is given below:

$$\gamma(h) = \begin{cases} \tau^2 + \sigma^2\left(\dfrac{3|h|}{2\theta} - \dfrac{|h|^3}{2\theta^3}\right) & |h| \le \theta \\ \tau^2 + \sigma^2 & |h| > \theta \end{cases} \tag{7}$$

2.5. Spatial interpolation techniques

2.5.1. Ordinary kriging

Spatial interpolation techniques are widely used for the estimation and prediction of spatial data. Ordinary kriging (OK) is the most preferred and common technique for this purpose [39]. This technique is based on the assumption that the mean is constant but unknown and provides unbiased estimation with minimized error variance [38]. The estimator of OK is defined as:

$$Z(x_0) = \sum_{i=1}^{n} W_i Z(x_i),\ \sum_{i=1}^{n} W_i = 1 \tag{8}$$

where $Z(x_0)$ is estimated measure at ungauged location x_0, W_i is weighting function for observed value $Z(x_i)$ and n represents the total number of sample data points in the study area.

The error variance is illustrated as;

$$\sigma^2 = \frac{\sum_{i=1}^{n}\left(Z(x_i) - Z(x_0)\right)^2}{n} \tag{9}$$

2.5.2. Inverse distance weighting

In IDW model, it is supposed that the sample points closer to predicted points have more effect on predicted value. So IDW assesses the predicted value by taking an average of all the known locations and allocating greater weights to adjacent points [40,41]. The IDW is described by the following formula:

$$Z(x_0) = \frac{\sum_{i=1}^{n} W_i Z(x_i)}{\sum_{i=1}^{n} W_i} \tag{10}$$

and

$$W_i = \frac{1}{h_i^k} \tag{11}$$

where k is the constant which decides how adjacent points affect the estimated value. A smaller value of k has a higher impact from distant points.

2.6. Cross-validation

The performance of the interpolation method was evaluated through cross-validation statistics. Several cross-validation statistics were widely used to assess the validity of interpolation methods (OK and IDW), including mean error and root mean square error [38,42]. These statistics can be calculated by mathematical equations:

$$\text{ME} = \frac{1}{n}\sum_{i=1}^{n}\left[Z(x_i) - Z^*(x_i)\right] \tag{12}$$

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left[Z(x_i) - Z^*(x_i)\right]^2} \tag{13}$$

where $Z^*(x_i)$ is the estimated measure of the same location. A model with the least value of ME and RMSE is considered the best model.

2.7. Water quality index

WQI is used to examine the quality of groundwater for drinking purposes [43]. For the calculation of WQI, firstly each water quality parameter has been assigned a weight (Table 2) according to their perceived effects on primary health [44] and then calculate the relative weights (W_i^*) for each parameter using:

$$W_i^* = \frac{w_i^*}{\sum_{i=1}^{n} w_i^*} \tag{14}$$

where W_i^* is the weights of each water quality parameter and n is the total number of parameters. After calculating the relative weights, the quality rating scale (q_i) was calculated for each parameter by the following formula:

$$q_i = \frac{c_i}{s_i} \tag{15}$$

where c_i is the concentration value for each water quality parameter and s_i is the standard value for each parameter (Table 2). The WQI can be measured by the following equation:

$$\text{WQI} = \frac{\sum_{i=1}^{n} \left(W_i^* \times q_i \right)}{\sum_{i=1}^{n} W_i^*} \tag{16}$$

3. Results and discussion

3.1. Descriptive analysis

The physiochemical and descriptive analysis of groundwater quality parameters including total dissolved solids (TDS), calcium (Ca), magnesium (Mg), hardness, sodium (Na) and sulfate (SO_4) from 105 locations of District Sheikhupura, Pakistan are presented in Table 1. We used R-Language and ArcGIS 10.7 software for descriptive and geostatistical analysis. Results from the Shapiro–Wilk normality test (Table 1) showed that all water quality parameters were non-normal and the coefficient of skewness also confirms the results. Box–Cox transformation was applied to normalize the water quality parameters. The range of TDS is from 134 to 2,094 mg/L with a mean value of 722.83 mg/L whereas the permissible limit according to WHO is 1,000 mg/L. Calcium and magnesium concentrations were under the permissible limits as shown in Table 1. The parameter hardness ranges from 78 to 600 mg/L with permissible limits less than 500 mg/L which shows that most of the location values were beyond the permissible limits. The water quality parameter sodium reaches up to 612 mg/L as its permissible limit is 200 mg/L and sulfate was also ranges wildly from 14 to 490 mg/L.

3.2. Parameter estimation of the experimental variogram

Geostatistical prediction based on the experimental variogram parameters (sill, range and nugget). The values of these parameters were estimated by using well-known estimation techniques like ordinary least square (OLS), maximum likelihood (ML) and restricted maximum likelihood (REML) with the assistance of variogram models including exponential, spherical, matern and Gaussian. Parameters were estimated by using the eyefit command in the GeoR package in R-language [45]. The best fitted theoretical model for the variogram of each parameter (TDS, CA, MG, hardness, Na and sulfate) was listed in Table 3. Moreover, cross-validation statistics are measured for the model of each parameter. Results showed that the ML estimation technique and spherical model were best fitted for TDS based on MSE. The matern variogram model was best fitted for Ca and Mg with the REML estimation technique. The spherical model was considered best for hardness and sulfate (Table 3). For sodium concentration, REML and exponential model were considered best.

The predictive performance of theoretical models for water quality parameters was determined through cross-validation statistics. Mean error and root mean square error were calculated to check the validity of interpolation methods (IDW and OK). It was observed from Table 4 that water quality parameter TDS have minimum values of ME and RMSE (2.43, 14.56) for OK rather than IDW. Calcium, magnesium, hardness and sodium also depict the lowest values of ME and RMSE for OK (Table 4). The only sulfate shows the larger value of ME and RMSE for OK as compared to IDW. Results show that the OK interpolation method performed better than IDW [46,47] based on ME and RMSE.

The spatial distribution of TDS concentration by OK interpolation method is shown in Fig. 2 (top left panel) and

Table 2
Relative weights for each water quality parameters

Parameters	WHO Standard	Pakistan Standard	Weight (w_i)	Relative weight (W_i)
TDS, mg/L	≤1,000	1,000	5	0.2083
Calcium, mg/L	≤250	200	3	0.125
Magnesium, mg/L	≤150	100	3	0.125
Hardness, mg/L	≤500	500	4	0.1667
Sodium, mg/L	≤200	200	4	0.1667
Sulfate, mg/L	≤250	200	5	0.2083

Table 3
Semivariogram parameters of best fitted theoretical model for water quality parameter

Groundwater parameters	Best-fitted model	Estimation method	Sill (σ^2)	Range (ϕ)	Nugget (τ^2)	MSE
TDS	Spherical	ML	0.57	0.38	0.68	200.16
Calcium	Matern	REML	0.22	0.17	0.13	23.01
Magnesium	Matern	REML	2.80	0.16	3.54	10.89
Hardness	Spherical	OLS	3.51	0.01	4.25	95.62
Sodium	Exponential	REML	14.78	0.28	6.68	47.53
Sulfate	Spherical	REML	6.39	1.99	0.33	53.05

MSE: Mean Square Error

Table 4
Cross-validation statistics for interpolation techniques

Parameters	Ordinary kriging		IDW	
	ME	RMSE	ME	RMSE
TDS	2.43	14.56	2.91	16.03
Calcium	3.87	7.08	4.17	7.38
Magnesium	1.65	4.59	3.21	4.89
Hardness	4.21	9.08	5.56	9.92
Sodium	0.76	3.87	1.09	4.76
Sulfate	1.97	7.51	1.33	7.19

ME: Mean Error; RMSE: Root Mean Square Error

it was assessed that TDS values were exceeding the permissible limits in the southwest part of the study area. It was observed that the Ca concentration was very high in 75% of the study area (Fig. 2) which is evident that the groundwater is contaminated in Sheikhupura. The increased level of Ca in groundwater may cause cancer. The interpreted groundwater quality concerning magnesium and hardness indicates that more than 65% study area lies in the range where the water is not suitable for drinking (Fig. 2). The larger values of magnesium and hardness impact human health and may cause laxative effects and cancer [48]. It is observed from Fig. 2 (bottom left panel) that the area with latitude 31.55°–31.66° and longitude 73.79°–73.93° have a very poor quality of groundwater. The spatial distribution map (Fig. 2 bottom right panel) of sulfate shows that most groundwater samples were unsuitable for drinking.

3.3. Estimation of water quality index

The water quality index is a useful technique for estimating the overall quality of the groundwater data [49], [50]. For the calculation of WQI, firstly each water quality parameter has been assigned a weight (Table 2) according to their perceived effects on primary health [50] and then calculate the relative weights (W_i) for each parameter. Quality rating scale (q_i) was calculated for each parameter and finally, WQI for every 105 locations was estimated. Estimated WQI values were classified into five categories Excellent, good, poor, very poor and unsuitable for drinking (Table 5). The excellent quality of groundwater is found in very small part (only 10 locations out of 105) of the study area which revealed that the quality of groundwater in District Sheikhupura is very poor and causes skin diseases and cancer. However, 36.2% of locations were found with good water. Eight locations were found where the water is unsuitable for drinking and at 12 locations the quality of water is very poor. On the whole, at 57 (55% of the study area) sampling locations the quality of groundwater is poor and from the rest, 45% only 9.6% of locations have excellent water for drinking. From Fig. 3, it is observed that the left bottom area with latitude 31.55°–31.66° and longitude 73.79°–73.93° have a very poor quality of groundwater. It is evident from the results of this study that the quality of groundwater is not satisfactory in Sheikhupura, Pakistan.

4. Conclusion

The present study was designed to elaborate on the use of interpolation methods (IDW and OK) for predicting the water quality parameters in Sheikhupura, Pakistan. The concentration of water quality parameters including TDS, Ca, Mg, hardness, Na and SO_4 were found exceeding the WHO permissible limits. It was assessed that TDS values were exceeding the permissible limits in the southwest part of the study area and Ca concentration was very high in 75% of the study area which is evident that the groundwater is contaminated in Sheikhupura. The increased level of Ca in groundwater may cause cancer. The interpreted groundwater quality concerning magnesium and hardness indicates that more than 65% study area lies in the range where the water is not suitable for drinking the larger values of magnesium and hardness impact human health and may cause laxative effects and cancer. It was observed that the area with latitude 31.55°–31.66° and longitude 73.79°–73.93° have a very poor quality of groundwater. After descriptive measures, the estimated parameters of the variogram were plugged into the prediction techniques for interpolation. Cross-validation measures showed that OK gives better prediction as compared to IDW. Concentration maps of TDS, Ca, Mg, Na, hardness and SO_4 showed the lower quality of water in different parts of the study area.

To show the combined effect of all water quality parameters, the WQI was used to prepare the map of the overall water quality of the study area. It was observed that the area (South-West) with latitude 31.55°–31.66° and longitude 73.79°–73.93° have a very poor quality of groundwater. It is evident from the results of this study that the quality of groundwater is not satisfactory in Sheikhupura, Pakistan. The rapid increase in population and industrialization are found to be the major cause of water contamination. Hence mitigation and preventive measures are required to

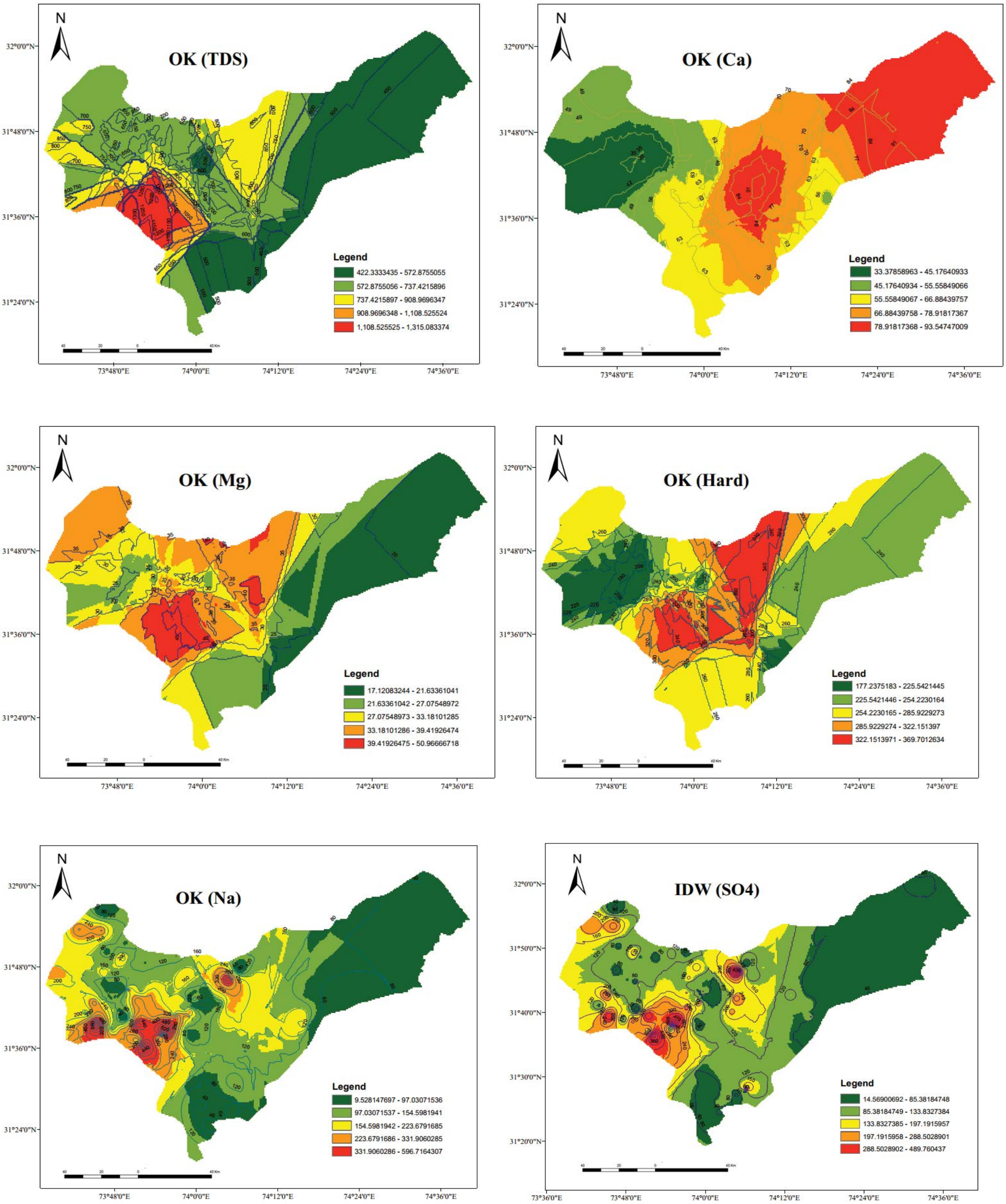

Fig. 2. Prediction maps using the best-fitted model for (TDS, Ca, Mg, hardness, Na and SO_4).

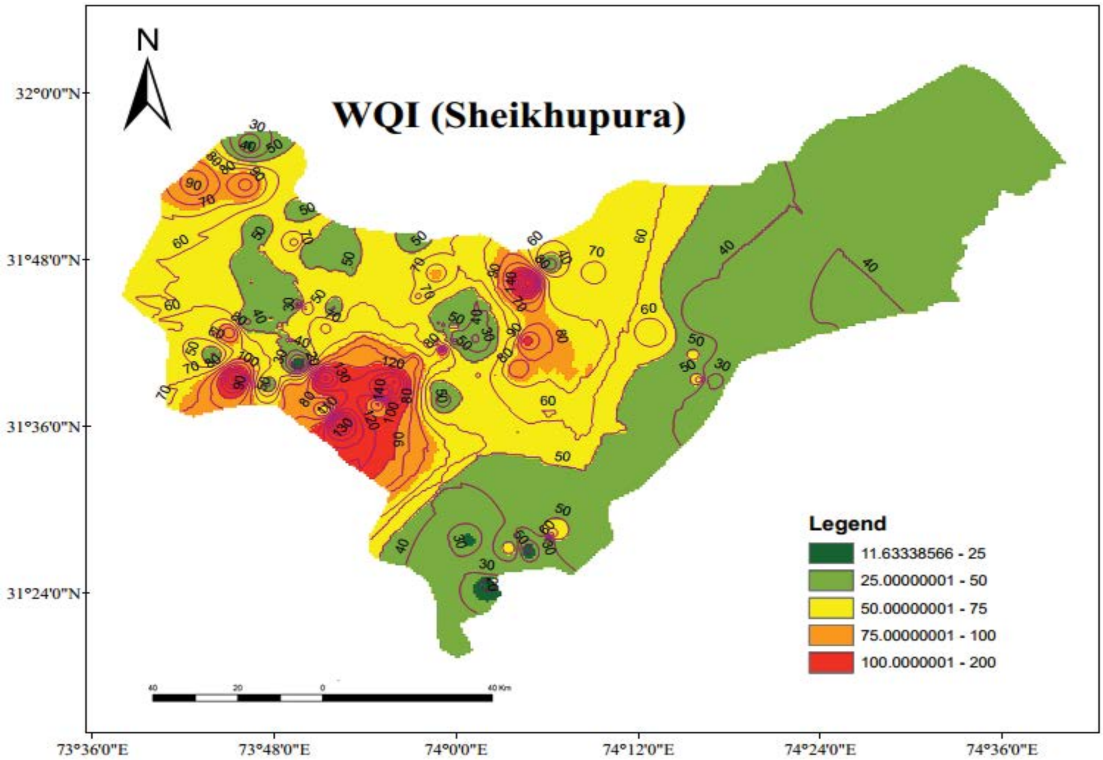

Fig. 3. Groundwater quality map of the study area by water quality index.

Table 5
Water quality status in District Sheikhupura

WQI Value	Water quality status	Samples lies	% Sample
Below 25	Excellent	10	9.6%
26–50	Good	38	36.2%
50–75	Poor	37	35.2%
75–100	Very poor	12	11.4%
Above 100	Unsuitable for drinking	8	7.6%

reduce the possible threat to human and ecological health. So it is recommended to the residents of this area to avoid groundwater without purification and the government should install water purification plants to save the lives of these residents.

Supplementary material

The data used in this study, accessible at the Pakistan Council of Research in Water Resources (PCRWR) by using this link http://www.pcrwr.gov.pk/publication.php?view_quality.

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