International Research Journal of Applied and Basic Sciences

ISSN 2251-838X / Vol, 4 (12): 3623-3632
Science Explorer Publications

Investigating spatio-temporal variability of groundwater quality parameters using geostatistics and GIS

Masoomeh Delbari[*1], Masoud Bahraini Motlagh[2], Milad Kiani[2], Meysam Amiri[2]

1. Assistant Professor, Department of Water Engineering, Faculty of Water and Soil, University of Zabol, Zabol, Iran
2. M.Sc. students of water resources Engineering, Department of Water Engineering, Faculty of Water and Soil, University of Zabol, Zabol, Iran

***Corresponding Author email:**mas_delbari@yahoo.com

ABSTRACT: Mapping the spatio-temporal distribution of water quality parameters is a crucial step in optimum utilization of groundwater resources. In this study we use information of 172 pizometric wells in Shiraz city, southern Iran to investigate the spatial variability of groundwater quality parameters (EC, SAR, TDS and Na) in 2005 and 2009. In order to do so, first the experimental semivariograms of selected parameters are calculated using GS^+ software and the best semivariogram models are fitted to the experimental data. The results showed that groundwater quality data are strongly spatially correlated over the study region. Spatial structure of all parameters except SAR 2005 follow a spherical model. For SAR in 2005 a Gaussian model is the best semivariogram model. Kriging approach via ArcGIS software is used to interpolate and map groundwater quality parameters. Groundwater qualitative map for agricultural purpose is produced through combining EC and SAR estimation maps considering US salinity laboratory standard. According to the generated maps, eastern parts have higher concentration of EC, TDS and SAR than other parts of the study area that could be duo to existence of salt lake there. The results showed that groundwater quality has slightly decreased from 2005 to 2009.
Key words: Spatial correlation; semivariogram; groundwater; EC; SAR; mapping; classification; USSL standard

INTRODUCTION

Inappropriate use of agricultural and irrigation facilities or designing faulty drainage for irrigation systems in Iran result in entering huge amounts of agricultural waste to water resources every year. The wastewater coming through rivers and drainage systems causes pollution and salinity problem in most water resources across the country. Because of the geologically saline nature of soil in many dry lands in Iran, sometimes saline waters exist naturally. Expansion of salinity in the Iranian plateau is not confined to salt-covered areas, salt swamps and saline aquifers; rather, the main problem is the existence of geologic systems containing evaporative deposits like gypsum and salt which can be seen in most regions over the country (Alizadeh, 2004). Generally, salt deserts are the main source of the salt distribution. Water movement and probably existence of winds on the surface and penetration of saline water into the interior layers of these deserts spread salinity in adjacent areas. Runoff over the basin becomes saline by passing through these areas. This process decreases not only the quality of potable and agricultural water, but also contaminates downstream areas and creates secondary deserts.

Entrance of pollution into water resources can significantly decrease surface and groundwater quality. Surface water and groundwater quality degradation are threats facing agricultural development over the country, especially in arid regions. Therefore, it is very important to estimate the spatial distribution pattern of water quality parameters for taking preventative actions and avoiding utilization of polluted water. Using Geographical Information System (GIS) and geostatistics it is possible to map water pollutants and improve qualitative and quantitative management of water resources (Balakrishnan, 2011). The basic idea in geostatistics is that data closer to each other are more similar than those farther apart (Isaaks and Srivastava, 1989). The spatial correlation between data points can be quantified by calculating a semivariogram. A semivariogram model is then used in kriging to interpolate the property of interest over the study region. Geostatistical approaches have been used for modeling the spatial distribution of many regional variables including groundwater quality parameters (Istok and Cooper, 1998; Lieu et al., 2004; Demir et al., 2009). Rizzo and Mouser (2000) used geostatistics to analyze groundwater quality data. Investigated parameters were sulfate, chloride, calcium, sodium and salinity. They used microbe population as auxiliary variable in cokriging method. Their results revealed that cokriging is a suitable approach for estimating groundwater quality parameters. Ahmed (2002) used kriging as an efficient tool for estimating water qualitative variables like Total Dissolved Solid (TDS). Ahmadi and Sedghamiz (2008) used kriging and cokriging (with using height as secondary variable) methods for preparing maps of groundwater depth in Darab desert in south of Fars Province, Iran. The results of geostatistical analysis revealed that the spatial variability of groundwater level varies for different climatic situations. They also calculated RMSE and showed that cokriging method is the most accurate approach in estimating groundwater depth. Demir et al. (2009) investigated the spatial variability of groundwater depth and salinity in northern Turkey. Sun et al. (2009) compared IDW, radial basis functions and kriging methods for predicting spatio-temporal variability of groundwater depth in China. They found ordinary kriging as the best interpolator. Delgado et al. (2010) used kriging to map groundwater quality parameters in Yukatan, Mexico. Based on the generated maps, they classified the study area into different zones in terms of water quality for agricultural uses. Adhikary et al. (2010) analyzed spatial variability of groundwater quality in India. They produced probability maps of groundwater contaminants using indicator kriging. Houshmand et al. (2011) used cokriging and kriging methods for spatial estimation of Sodium Absorption Ratio (SAR) and Chloride (Cl) concentration in groundwater. For SAR and Cl data, Gaussian model was proved to be the best semivariogram model. Kriging methods were also used by Rawat et al. (2012) to predict spatial distribution of some groundwater quality parameters. Balakrishnan (2011) used GIS spatial interpolation technique to map the groundwater quality information over a study area in India.

The aim of this research is to estimate and classify groundwater quality of Shiraz city, south of Iran for agricultural purposes. Kriging and cokriging approaches are used for estimating properties under study and classification is performed based on USSL classification diagram within GIS environment.

MATERIALS AND METHODS

Study region

Fars province is located in south of Iran between 50 and 55 degrees east longitude and 27 and 31 degrees north latitude. Having an area of 122608 square kilometers, the province is the fifth largest province in the country and occupies almost 1.8 percent of Iran. This research was conducted in the capital of Fars province, Shiraz (Figure 1). Shiraz city is geographically placed on 52° 32' east longitude and 29° 36' north latitude. The township has an area of 10479 square kilometers and an altitude of 988 to 3098 meters. Long-term (40 years) annual rainfall is 330 millimeters and long-term average temperature is 17.9 degrees Celsius. The township is divided to six parts, seven cities including Shiraz, 22 rural districts and 811 villages.

Groundwater quality data

Groundwater samples have been taken from 172 pizometric wells for some successive years. Well locations are shown in Figure 1. For each sample, latitude and longitude of wells were recorded using the Global Positioning System (GPS). In this study we used qualitative data obtained in 2005 and 2009. Target parameters are Electrical Conductivity (EC), SAR, TDS and sodium (Na). EC and SAR are very important in classifying waters from the agricultural viewpoint. EC indicates the total amount of dissolved ions in the water, while SAR is a measure of the relative preponderance of sodiumdissolved in water compared to the amounts of dissolved calcium and magnesium. SAR can be calculated using the following equation:

$$SAR = \frac{cNa}{\sqrt{\frac{(cCa+cMg)}{2}}} \quad (1)$$

where cNa is sodium concentration (meq/lit), cCa is calcium concentration (meq/lit) and cMg is magnesium concentration (meq/lit).

According to the equation (1), SAR increases as a result of increasing sodium content relative to calcium and magnesium concentrations. High amount of sodium ions in water causes infiltration problems and affects the

permeability of soil. So it results in less water uptake by plant roots. An increase in sodium may cause other problems to the crop such as the formation of crusting seed beds, temporary saturation of the surface soil, high pH and the increased potential for diseases, weeds, soil erosion, lack of oxygen and inadequate nutrient availability.
In this study water quality classification is performed using USSL diagram (Figure 2). In this diagram, C and S denote EC and SAR, respectively. Classification of irrigation water quality based on C and S are presented in Tables 1 and 2, respectively. Accordingly, in Figure 2, C_1S_1 indicates very good quality, C_1S_2, C_2S_2 and C_2S_1 indicate good quality, C_1S_3, C_3S_1, C_3S_2, C_3S_3 and C_2S_3 indicate medium quality and the others indicate poor quality of irrigation water for agriculture (USSL, 1954).

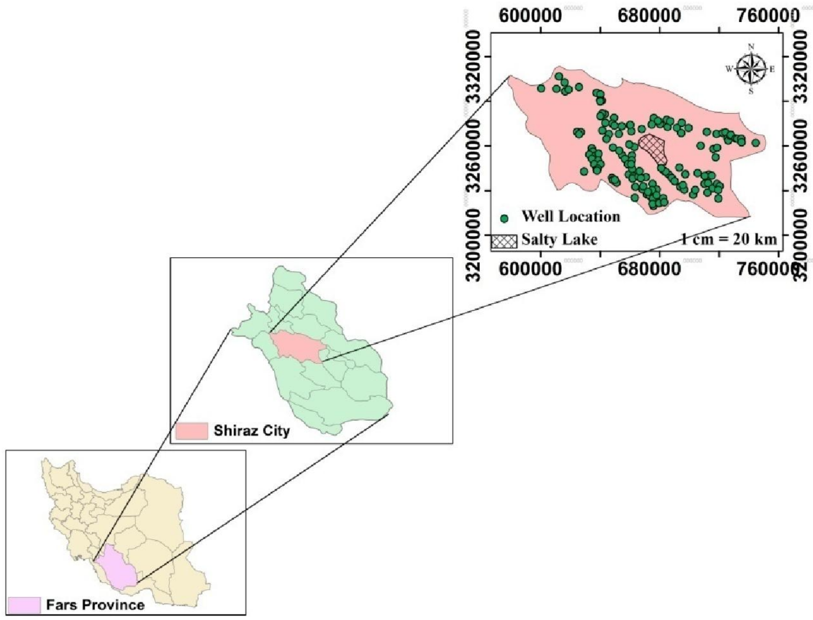

Figure 1. Location map of the study area and pizometric wells

Table 1. Classification of irrigation water quality based on EC

EC(µmhos/cm)	Class	Salinity hazard
100-250	C_1	Low
250-750	C_2	Medium
750-2250	C_3	High
>2250	C_4	Very High

Table 2. Classification of irrigation water quality based on SAR

SAR	Class	Sodicity hazard
<10	S_1	Low
10-18	S_2	Medium
18-26	S_3	High
>26	S_4	Very High

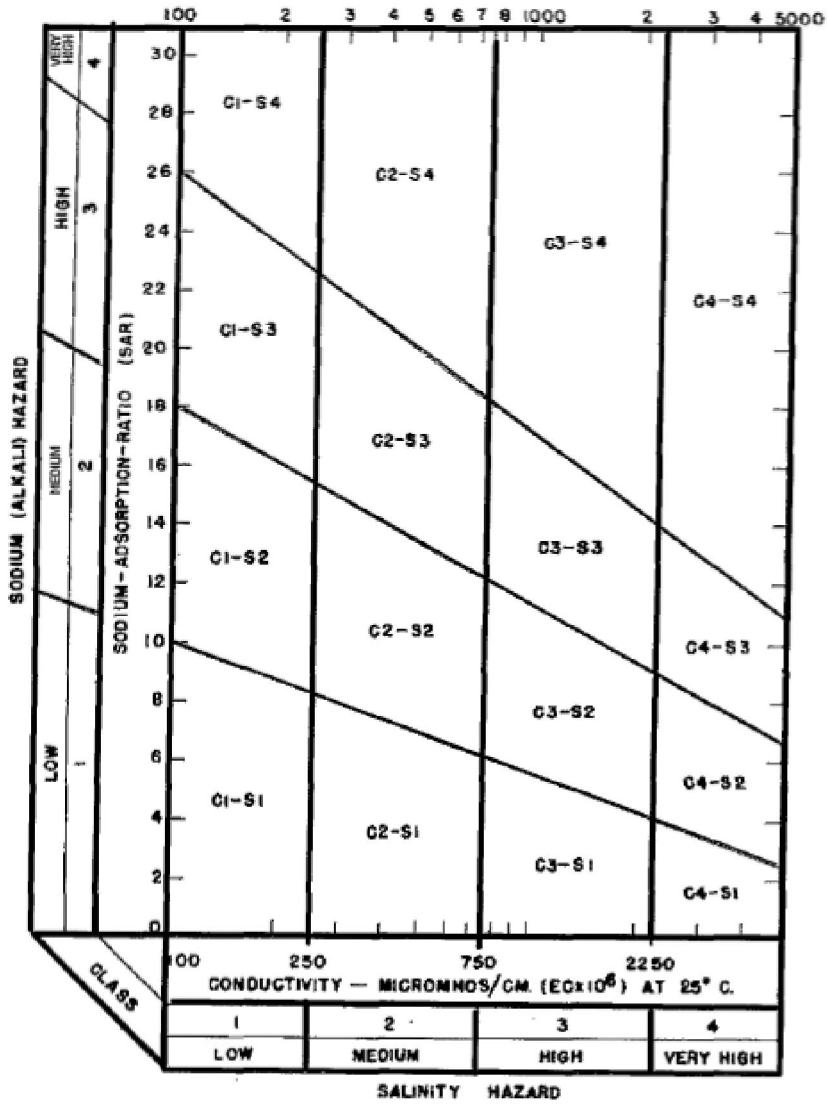

Figure 2. USSL diagram for irrigation water quality classification (USSL, 1954)

Geostatistics

The theory of geostatistics has been explained by many researchers including Isaaks and Srivastava (1989) and Goovaerts (1997).

Variogram is one of the most important tools for quantifying spatial correlation between data points. Variogram is actually the variance of data values in two points separated by h distance from each other. In practice experimental semivariogram and cross-semivariogram are used to investigate the spatial (cross) correlation between data values (Isaaks and Srivastava, 1989):

$$\gamma_{zs}^{*}(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} \left\{ \left[z(x_i + h) - z(x_i) \right] \left[s(x_i + h) - s(x_i) \right] \right\} \quad (2)$$

where, γ_{zs}^{*} is the experimental semivariogram when z=s and cross-semivariogram when $z \neq s$and N(h) indicates pairs of random variables $z(x_i)$ and $s(x_i)$ separated by a lag distance h.

After calculating experimental (cross) semivariogram, a theoretical model should be fitted to the experimental data. The most common semivariogram models are spherical, exponential and Gaussian models. Spherical and Gaussian models used in this study are expressed as following (Isaaks and Srivastava, 1989):

$$\gamma(\mathrm{h}) = \begin{cases} \mathrm{C_0} + \mathrm{C}\left[\frac{3}{2}\frac{\mathrm{h}}{\mathrm{a}} - \frac{1}{2}\left(\frac{\mathrm{h}}{\mathrm{a}}\right)^3\right] & \mathrm{h} \le \mathrm{a} \\ \mathrm{C_0} + \mathrm{C} & \mathrm{h} > a \end{cases} \quad \text{spherical model} \qquad (3)$$

$$\gamma(\mathrm{h}) = \mathrm{C_0} + \mathrm{C}\left(1 - \mathrm{e}^{-\frac{\mathrm{h}^2}{\mathrm{a}^2}}\right) \quad \text{Guassian model} \qquad (4)$$

where C_0 is the nugget effect, C_0+C is sill and a is the range of influence. After fitting the model, (cross) semivarigram characteristics will be used in kriging system of equations in order to interpolate the desired variable.

Ordinary Kriging

Ordinary kriging (OK) is the most commonly used geostatistical interpolation method. OK estimator, also called the best linear unbiased estimator (BLUE), can be defined as follows (Journel and Huijbregts, 1987):

$$z^*(x_0) = \sum_{i=1}^{n} \lambda_i \cdot z(x_i) \quad with \quad \sum_{i=1}^{n} \lambda_i = 1 \qquad (5)$$

where $z^*(x_0)$ is the estimated value for the variable at location x_0, $z(x_i)$ is the observed value at location x_i and $\lambda_i$is the weight assigned to the neighboring observation $z(x_i)$. OK weights are obtained by solving the following equations:

$$\begin{cases} \sum_{j=1}^{n} \lambda_j \gamma(x_i - x_j) + \mu = \gamma(x_i - x_0) \quad i = 1,...,n \\ \sum_{j=1}^{n} \lambda_j = 1 \end{cases} \qquad (6)$$

where μ is the Lagrange multiplier. Kriging provides optimum results in presence of normal distribution of data. When data distribution is not normal, an appropriate transformation of data should be used beforehand. In case of log normal transformation, kriging used on transformed data is called log normal kriging.

Cokriging

In cokriging (COK) one or more secondary variables, which are correlated with the main variable are used for the interpolation. It is supposed that these secondary variables can improve the accuracy of the estimation. COK estimator is defined as (Goovaerts 1997):

$$z^*(x_0) = \sum_{\alpha=1}^{n} \lambda_\alpha \cdot z(x_\alpha) + \sum_{\beta=1}^{m} \lambda_\beta \cdot s(x_\beta) \qquad with \quad \sum_{\alpha=1}^{n} \lambda_\alpha = 1 \quad \sum_{\beta=1}^{m} \lambda_\beta = 0 \qquad (7)$$

Where λ_α and λ_β are the weights assigned to the known values of the primary and secondary variables z and s, respectively and n and m are the number of primary and secondary observations. The weights are determined through COK system of equations similar to OK (Goovaerts, 1997).

Comparison of interpolation methods

A cross-validation (Isaaks and Srivastava, 1989) approach is used to assess the performance of OK and COK. The comparison criteria used are mean bias error (MBE), root mean square error (RMSE) and determination coefficient (R^2). Mathematical formula for MBE and RMSE are given as:

$$MBE = \frac{1}{N}\sum_{i=1}^{N}\left[z^*(x_i) - z(x_i)\right] \quad (8)$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left[z^*(x_i) - z(x_i)\right]^2} \quad (9)$$

where $z^*(x_i)$ and $z(x_i)$ are the estimated and observed values at location x_i, respectively and N is the number of observations. For an appropriate estimator, MBE should be close to zero, R^2 should be close to 1 and RMSE should be as small as possible.

RESULTS AND DISCUSSION

Statistical analysis

Table 3 provides descriptive statistics for EC, SAR, Na and TDS data in 2005 and 2009. The minimum, maximum and mean values for EC, SAR and TDS increase from 2005 to 2009 while Na does not change too much over these years. Statistical analysis shows that the coefficient of variation is very high (above 100%) for EC, SAR and TDS in two investigated years. This suggests that EC and SAR changes dramatically over the study region. This is due to existence of a salt lake in the center of Shiraz Township which results in a high level of salinity in the adjacent groundwater. The frequency distributions of all investigated parameters are positively skewed. So the data are transformed using a log transformation function. The skewness coefficient of transformed data (Table 3) is much less than those of real data and the frequency distribution curves are almost normal (not shown). Statistical analysis showed that there is a strong correlation between groundwater quality parameters. Therefore TDS and Na are used as secondary variables to possibly improve the estimation accuracy of EC and SAR, respectively and vice versa.

Table 3. Summary statistics of groundwater quality data

Parameter	year	mean	Min	max	SD*	CV** (%)	Skewness
EC(µm/cm)	2005	2489.1	275	14130	2799	112.45	1.99
	2009	3300.3	342	18715	5622.4	170.36	2.86
Log EC	2005	7.44	5.62	9.56	0.93	12.50	0.27
	2009	7.58	5.80	10.90	1.06	13.98	0.51
SAR	2005	2.67	0.04	27.15	4.41	165.17	2.84
	2009	3.27	0.15	46.79	5.82	177.98	3.89
Log SAR	2005	0.19	-3.20	3.30	1.27	668.42	0.51
	2009	0.44	-1.9	3.85	1.24	281.82	0.49
Na(meq/lit)	2005	23.29	1.63	78.56	17.77	76.30	1.37
	2009	24.90	2.49	70.13	16.10	64.66	0.89
Log Na	2005	2.89	0.49	4.36	0.7	24.22	0.09
	2009	2.30	0.91	4.25	0.69	22.00	-0.20
TDS	2005	1655	196	8330	1752	105.86	1.74
	2009	2156	224	11400	2542	117.90	2.02
Log TDS	2005	6.94	5.28	9.03	0.96	13.83	0.32
	2009	7.13	5.41	9.34	1.02	14.31	0.40

*Standard deviation

**Coefficient of Variation

Spatial variability analysis

To investigate the spatial variability of groundwater quality parameters, experimental semivariogram of data values are calculated in four directions 0, 45, 90 and 135 degrees with an angle tolerance of 22.5 degree. The results show no significant anisotropy, hence the investigated parameters are assumed to be isotropic and omnidirectional semivariogram is calculated for each of them. Then the best semivariogram model is fitted to the experimental data. Semivariogram model characteristics for each water parameter are given in Table 4. The best model is the one having least residual sum of squares (RSS) and largest regression coefficient (R^2). As suggested by many researchers such as Camberdella et al. (1994) when the value of $C_0/(C+C_0)$ in Table 4 is less than 0.25, the variable has a strong spatial correlation. The results revealed that spatial structure of all variables except SAR 2005 follow a spherical model. The best semivariogram model for SAR 2005 is Gaussian. Experimental cross semivariograms are also calculated and modeled for using in COK system. The results are given in Table 4.

Table 4. Characteristics of semivariogram models for groundwater quality parameters

Parameter	Model type	C_0	C_0+C	C_0/(C+C_0)	Effective Range (m)	R^2	RSS
EC 2005	Spherical	0.20	0.80	0.25	25800	0.97	0.006
EC 2009	Spherical	0.19	0.85	0.22	26200	0.93	0.053
SAR 2005	Gaussian	0.52	1.44	0.36	23729	0.93	0.068
SAR 2009	Spherical	0.25	1.087	0.23	27700	0.91	0.092
TDS 2005	Spherical	0.24	0.81	0.29	25400	0.92	0.060
TDS 2009	Spherical	0.23	0.91	0.25	26400	0.93	0.024
Na 2005	Spherical	0.60	2.25	0.27	26300	0.92	0.17
Na 2009	Spherical	0.17	0.347	0.49	32200	0.84	0.007
Na-SAR(2005)	Spherical	0.449	1.775	0.26	26500	0.98	0.010
Na-SAR(2009)	Spherical	0.21	0.577	0.36	36500	0.92	0.008
TDS-EC (2005)	Spherical	0.197	0.728	0.27	25100	0.96	0.008
TDS-EC (2009)	Spherical	0.207	0.885	0.23	26200	0.936	0.021

Spatial prediction of groundwater quality parameters

The semivariogram model characteristics given in Table 4 are used in OK and COK to interpolate the groundwater quality parameters over the study region. The cross validation results of estimating groundwater quality parameters (Table 5) indicate that COK achieving a slightly smaller RMSE and higher R^2 performs better than OK. This means that using secondary variables even with the same size of the main variable improved the estimation accuracy of the main variable over the study region. This is in line with the results obtained by Rizzo and Mouser (2000) and Ahmadi and Sedghamiz (2008). Rizzo and Mouser (2000) identified cokriging as the best interpolation method in classification of water quality parameters including sodium, chlorine, sulfate, calcium and salinity. The results showed that cokriging is suitable for most groundwater parameters. The results of Ahmadi and Sedghamiz (2008) showed that cokriging method is more accurate than ordinary kriging in estimating groundwater depth.

Table 5. Cross validation results of estimating groundwater quality parameters using OK and COK

Parameter	OK			COK		
	MBE	RMSE	R^2	MBE	RMSE	R^2
EC 2005	36.89	2226	0.38	35.45	2198	0.40
EC 2009	9.82	2583	0.55	0.79	2111	0.56
SAR 2005	-0.01	3.53	0.39	0.07	3.52	0.40
SAR 2009	-0.15	4.37	0.44	-0.13	4.36	0.45
TDS 2005	35.39	1354	0.39	16.73	1354	0.40
TDS 2009	7.09	1740	0.53	18.13	1731	0.54
Na 2005	-0.19	3.53	0.40	0.07	3.52	0.40
Na 2009	-0.18	10.84	0.55	-0.31	10.85	0.55

In this study COK is used to produce the maps of the spatial distribution of EC, SAR, Na and TDS (Figure 3). Afterwards sampling point layer is superposed on the classification layer and expected values are compared with observed values. The results show that expected and observed values are highly correlated.

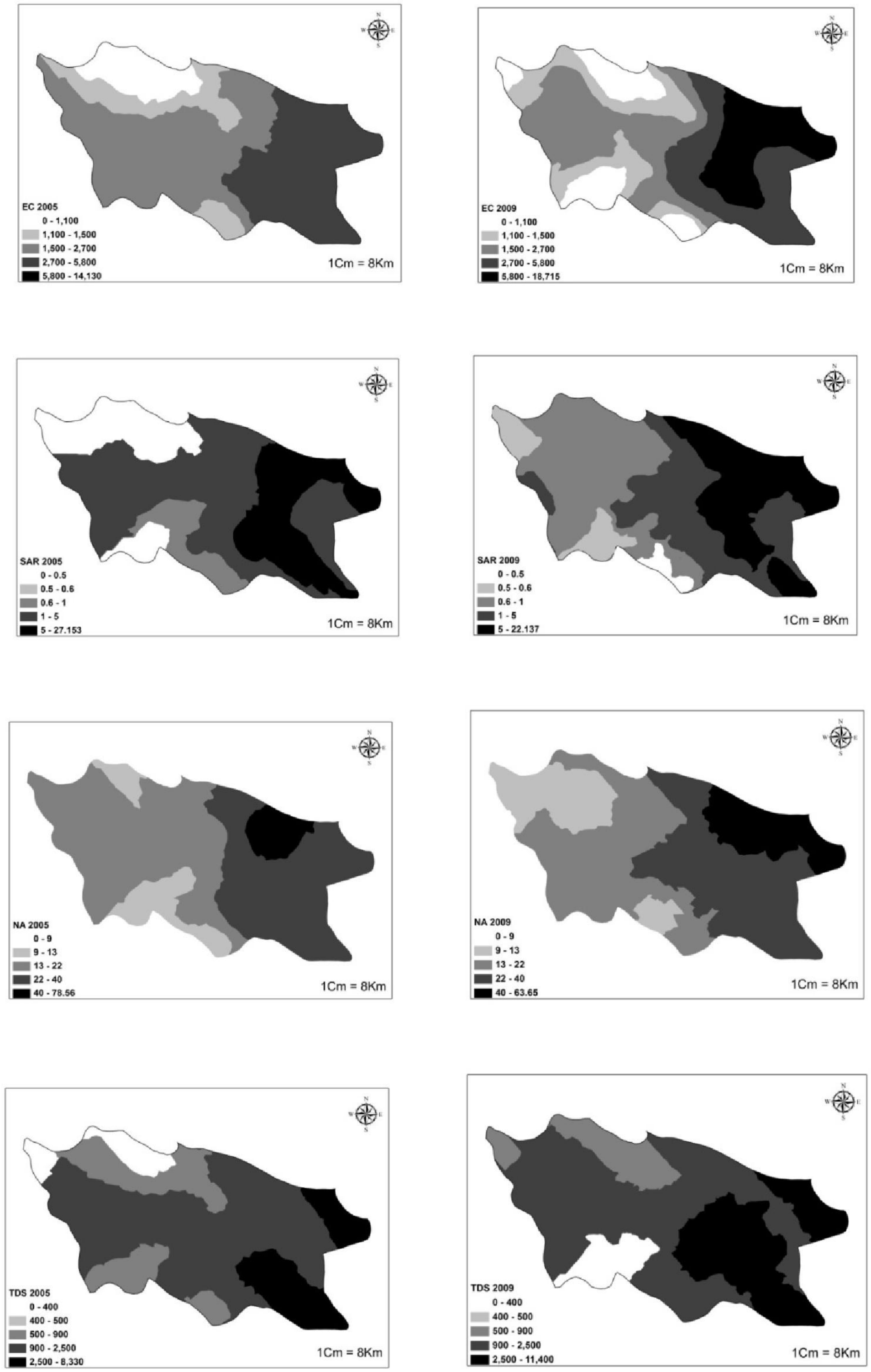

Figure 3. Mapping groundwater quality parameters using COK for 2005 and 2009.

In the next step we performed classification of the study area in terms of groundwater quality for irrigation based on USSL standard for the years 2005 and 2009 within the GIS media (Figure 4). The results reveal that in 2005 more than 91 percent of the study region fall into classes C3S1 and C4S1. Similarly in 2009, most of the study area belongs to C3S1 and C4S1 classes.

According to the generated maps (Figure 4), it can be seen that the quality of irrigation water in the south of Shiraz Township has improved from C3S1 in 2005 to C2S1 in 2009. In central areas, however, the portion of C3S1 class has decreased from 2005 to 2009. In a similar manner, a reduction in groundwater quality from C3S1 in 2005 to C4S1 in 2009 can be seen in some parts in western areas. According to Table 6, the area of C4S1 class is almost constant during four years of investigation, while the area of C3S1 class has decreased from 58.16% in 2005 to 45.8% in 2009. Moreover, the results (Table 6) indicate that the area of C4S2 class has increased from 0% in 2005 to 8% in 2009, which suggests small improvement of groundwater quality during four years. Last, the areas of C2S1 and C4S3 classes have slightly increased during 2005 to 2009.

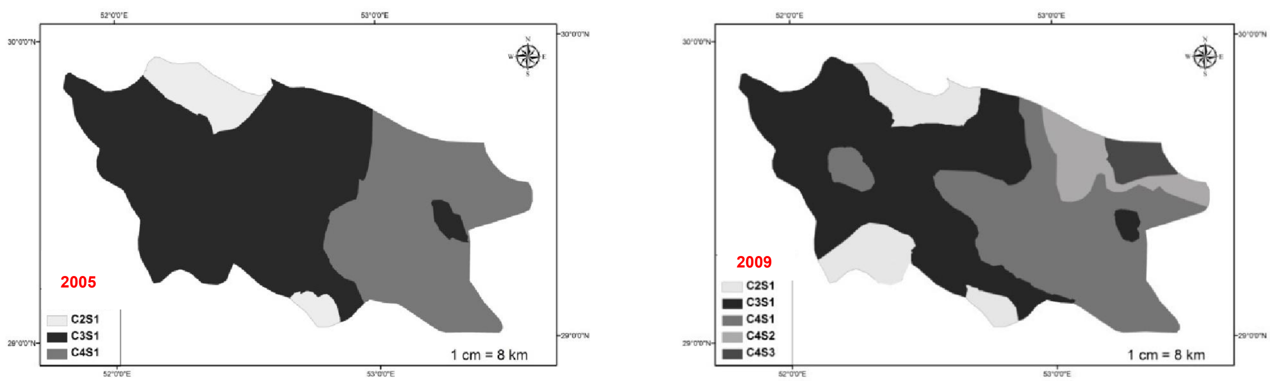

Figure 4. Classification of groundwater quality for irrigation based on USSL standard for 2005 and 2009.

Table 6. The estimated area for different water quality classes based on USSL standard

Class	Area in 2005 (%)	Area in 2009 (%)
C_2S_1	8.17	10
C_3S_1	58.16	45.8
C_4S_1	33.67	33.2
C_4S_2	0	8
C_4S_3	0	3

CONCLUSION

A geostatistical analysis is performed on groundwater quality data including EC, SAR, Na and TDS. Comparing OK and COK methods for interpolating groundwater quality parameters show that cokriging has a smaller RMSE and a higher R^2 than OK. Therefore, the maps for water quality classification were produced using cokriging within the GIS environment. According to provided maps, it was concluded that values of qualitative parameters are higher in eastern region which could be due to existence of a saline lake in eastern part of Shiraz Township. In this study a classification map of groundwater quality for irrigation uses is produced based on USSL standard for 2005 and 2009. Based on the maps generated, study area has some level of salinity problem towards eastern regions. However there is no sodicity problem across the study area.

Overall, water quality classification maps generated in this study should be used as a guideline to define appropriate management practices in irrigated agriculture to maintain existing soil productivity with the benefits of high crop yields under irrigation.

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