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Using geostatistical and deterministic modelling to identify spatial variability of groundwater quality

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Abstract

The main portion of water demands of arid regions like Kashan Plain, Iran supply by groundwater wells. This research was conducted to assess the groundwater quality as well as modelling and mapping groundwater quality in the study area using geosatistics and deterministic techniques. Five water quality parameters, including Electrical Conductivity, Sodium Adsorption Ratio, Total Hardness, Total Dissolved Solids and pH, were applied to determine the irrigation and drinking water quality index using the Wilcox diagram and WHO standards. The final map indicated that the groundwater quality increased from north to south of the study area. The areas located in the centre, south and eastern south of the study area had the optimum quality for irrigation and drinking purposes. Furthermore, based on the results of zoning using the Wilcox diagram determined that ground water quality of the study area 22%, 42% and 36% were good, medium and non-suitable, respectively.

Keywords: Groundwater quality; Modelling; Geostatistic; Deterministic; Zoning

1. Introduction

The usage of groundwater has gradually increased owing to increase of water demand and shortage of surface water during the growth of population and rapid industrialization, especially in arid and semi-arid regions (Nas, 2009; Belkhiri and SheikhiNarany, 2015; Bodrud-Doza *et al*., 2016). Water quality is closely linked to water use and to economic development status (Prabu *et al*., 2011; Karami *et al*., 2018). Groundwater can become contaminated with numerous types of human activities such as municipal, residential, industrial, commercial and agricultural usage (Keshtkar *et al*., 2016).
Iran Central Plateau is known as an arid to semi-arid region of the world, and most of fresh water is allocated for agriculture, is supplied through ground water (Babakhani *et al*., 2016; Keshtkar *et al*., 2017). Thus, it is clearly concluded that groundwater is the vital component for sustainable agriculture. In recent years, many fertile and agricultural plains suffered from 0.5 to 15 m water table-level drop (Ahmadi and Sedghamiz 2007; Sadat Noori, 2012), and most of water resources are gradually becoming polluted due to addition of materials from their surroundings (Lokeshwari and Chandrappa, 2006; Prabu *et al*, 2011) in which many wells are now out of use. Understanding the behaviour of groundwater body and its long-term trends is essential to make any management decisions in a given watershed (Reghunath *et al*., 2005; Sadat Noori, 2012). Therefore, having a deep knowledge about and insight into the groundwater system and evaluating the suitability of water quality seem necessary for optimum exploitation of water (Hu *et al*., 2005). The quality of irrigation water has to be evaluated to avoid or, at least, to minimize impacts on agriculture (Mohammed, 2011; Brhane, 2016).

Natural resources and environmental concerns, including groundwater, have considerably benefited from using GIS. An ArcGIS geostatistical analyst effectively bridges the gap between geostatistics and GIS analysis (Kumar *et al*., 2007; Nas, 2009; Kheradpisheh *et al*., 2014). Geostatistical analysis has been useful

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to determine water variables in spatial and temporal aspects, and water suitability for various purposes (Issaks *et al*., 1989; Goovaerts, 1997; Nas, 2009; Brhane, 2016; Mohammadi, 2017).

Many researchers applied geostatistical approach to analyse spatial variations of groundwater characteristics (Issaks *et al*., 1989; Bjerg *et al*., 1992; Ahmad, 2007; Nas, 2009, Abadi *et al*., 2016). Noori *et al*. (2013) compared different geostatistical methods to estimate a groundwater level at different climatic periods. Geostatistical methods were applied on the maximum, minimum and mean groundwater-level elevation of 59 wells. The results obtained from geostatistical analysis indicated that best method for this place was Cokriging, and groundwater depth varied spatially in different climatic conditions. Jeihouni *et al*. (2014) evaluated the groundwater quality of Tabriz city. The spatial distribution of groundwater quality parameters was produced by employing GIS and geostatistical techniques. Brhane (2016) evaluated groundwater by nine chemical parameters to calculate the irrigation water quality index. The results showed that groundwater suitable for irrigation purposes, and groundwater needed slight water treatment for quality adjustment. Laze *et al*. (2016) evaluated some significant physio-chemical parameters of the surface water of the Dukagjin Basin to assess the quality of irrigation water. The results suggest that all water samples are suitable for irrigation purposes. Mohammadi *et al*. (2017) evaluated the temporal and spatial variation of chemical parameter concentration in drinking water resources of Bandar-e Gaz city using GIS. According to the zoning maps of groundwater, nitrate and hardness concentration in dry seasons is greater than that in rainy seasons.

Kashan plain is located in an arid area of central Iran causing ecosystem conditions in this area to become extremely fragile. In recent decades, due to an intensive ground water usage, water quantity and quality were decreased. Thus, regarding the Kashan plain water resources condition, the main purpose of the current research was to evaluate geostatistical and deterministic techniques of groundwater quality modelling and calculate water quality indices in the study area.

2. Materials and Methods

2.1. The study area

The study is located north of Iran Central Plateau and Isfahan province, Iran. It has an area of 1741 km^2, and is located between a longitude of 33°30' - 34°30' N and latitude of 51°10' - 52° E (fig. 1). There is a waste pits in south of plain. The study area has an average annual rainfall of 122 mm with an average annual temperature of 18C°. According to Domarton method of climate classification study area is located in arid region. The study area has two modes of relatively different climatic; the two modes include climatic conditions foothill and lowland. A large proportion of water requirements for the city of Kashan are supplied from groundwater wells.

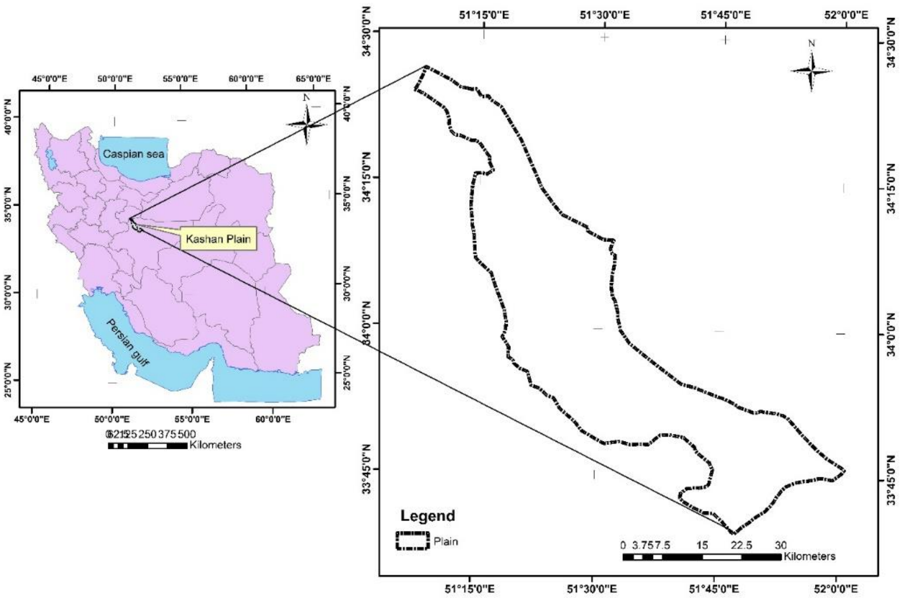

Fig. 1. Geographic location of Kashan plain

2.2. Groundwater quality data collection and analysis

Groundwater quality parameters were selected among many factors based on the significance of the parameter as an index for salinity, thereby affecting human health and data availability. Available groundwater of 72 observation wells monitored continually from 2000 to 2011 and received from Iran Water Resources Management Corporation was applied. These wells are distributed across the study area to represent the fluctuation of groundwater level and quality of the study area. The data of the ground water quality, including TH, EC, SAR, TDS and pH, were applied for the physical and chemical water quality analysis using standard classification methods (Table 1).

Table 1. Ground water quality parameters classification which applied for ground water quality analysis of Kashan plain

SAR	Quality	EC	Quality	TDS	Quality	TH	Quality	pH	Quality
0-10	Low	0-250	Low	<500	Suitable	<250	Suitable	<6	Acidic
10-18	Medium	250-750	Medium	500-1000	Tolerable	250-500	Tolerable	6-8	Neutral
18-16	High	650-2250	High	1000-2000	Unsuitable	500-1000	Unsuitable	>8	Alkaline
26-32	Very high	2250-4000	Very high	2000-4000	Inferior	1000-2000	Inferior		
				4000-8000	Temporality potable	2000-4000	Temporality potable		
				>8000	potable	>4000	potable		

The Wilcox classification was applied for quality comparison in terms of agriculture and irrigation (Soltani *et al*., 2014). The Wilcox diagram based on two factors of SAR, and EC classifies the samples in 16 different classes, that C_1S_1 and C_4S_4 with minimum and maximum salinity and alkalinity are the best and worst, respectively. In the Wilcox diagram, SAR shows the losses consequences by sodium. Maximum rate of sodium plays the main role of alkaline soil creation and eventually decreases soil permeability (Rahimi, 2009; Soltani *et al*., 2014).

2.3. Interpolation methods

Deterministic and geostatistical techniques are two main interpolation technique groups, which have been explained before in many manuscripts (Kumar *et al*., 2007; Nas, 2009; Sadat Nori *et al*., 2012; Kheradpisheh *et al*., 2014; Afzali *et al*., 2016; Babakhani *et al*., 2016). A geostatistical method is a branch of statistics focused on spatial patterns analysis and variables quantity assumption in points where sampling has not occurred. In this method, the variable and its spatial position are simultaneously used for spatial models. The main purpose of geostatic is to use notation change and other techniques in order to determine quantity and spatial correlation modelling.

In order to apply geostatistical methods, in the first step data normality was checked using maximum, minimum, average, median, standard deviation, the coefficient of skewness and kurtosis. Normalization using the logarithmic functions method was carried out if data failed to comply normal distribution. Then, according to the value of the errors calculated by the software, the best model was chosen that had the lowest root mean square error (RMSE) and maximum correlation (R) between existing data and estimated data. In this study, we tested four semivariogram models, including Circular, Spherical, Exponential and Gaussian.

Afterward, the normalization of the data interpolation was performed in IDW (Inverse Distance Weighting), RBF (Radial Basis Functions) and four geostatistical methods, including Ordinary Kriging, Simple Kriging, Cokriging Ordinary, and Cokriging Simple.

3. Results and Discussion

Tables 2 to 6 shows the summery of semivariogram model parameters for each water quality factor. As mentioned above, cross-validation was applied to determine which model prepared the best estimations (Table 2-6). The results of the error rate different methods, including IDW, RBF and four geostatic techniques (including Ordinary Kriging, Simple Kriging, Ordinary Cokriging and Simple Cokriging) were compared, then zoning of water quality was carried out using Gaussian Ordinary Kriging for electrical conductivity and Gaussian Simple Kriging for the sodium adsorption ratio, which according to the lowest error, they were identified as the best methods.

Table 2. Cross-validation results of Simple Kriging technique

Model	Parameter	Root Mean Square	Average Standard Error	R	Root Mean Square Standardized
Spherical	TH	468.8	410.5	0.62	1.15
	TDS	1444.14	1056.3	0.623	1.34
	pH	0.2475	0.253	0.598	0.9758
	EC	2328.21	-0.0735	0.67	1.3945
	SAR	2.491	-0.0112	0.62	1.0453
Circular	TH	466.76	418.54	0.642	1.107
	TDS	1423.93	1114.28	0.67	1.23
	pH	0.2474	0.2537	0.667	0.973
	EC	2289.21	-0.037	0.641	1.2658
	SAR	2.4606	0.01449	0.618	0.938
Exponential	TH	505.18	368.6	0.548	2.022
	TDS	1533.4	1354.4	0.623	1.10
	pH	0.248	0.2532	0.643	0.9726
	EC	2471.28	0.02608	0.672	1.0741
	SAR	2.6985	-0.0291	0.625	1.3754
Gaussian	TH	475.82	426.66	0.589	1.112
	TDS	1428.23	1145.69	0.595	1.23
	pH	0.247	0.2538	0.612	0.972
	EC	2291.76	-0.055	0.64	1.2936
	SAR	2.4576	0.0076	0.623	0.9192

Table 3. Cross-validation results of Ordinary Kriging technique

Model	Parameter	Root Mean Square	Average Standard Error	R	Root Mean Square Standardized
Spherical	TH	466.5	403.7	0.623	1.15
	TDS	1428.2	1223.7	0.618	1.15
	pH	0.251	0.243	0.650	1.03
	EC	2301.95	0.016	0.625	1.16
	SAR	2.524	0.0156	0.623	1.05
Circular	TH	465.7	400.26	0.625	1.15
	TDS	1431.3	1192.6	0.602	1.18
	pH	0.258	0.258	0.641	0.99
	EC	2310.9	0.017	0.630	1.18
	SAR	2.530	0.017	0.621	1.07
Exponential	TH	468.75	413.73	0.597	1.12
	TDS	1454.97	1158.5	0.581	1.25
	pH	0.2505	0.2456	0.601	1.02
	EC	2340.96	0.0156	0.660	1.20
	SAR	2.578	0.0163	0.628	1.05
Gaussian	TH	468.12	403.78	0.620	1.15
	TDS	1445.09	1186.3	0.640	1.20
	pH	0.2532	0.244	0.600	1.03
	EC	2326.55	0.0193	0.657	1.21
	SAR	2.575	0.0134	0.631	1.21

Table 4. Cross-validation results of Simple CoKriging technique

Model	Parameter	Root Mean Square	Average Standard Error	R	Root Mean Square Standardized
Spherical	TH	433.17	401.5	0.652	1.074
	TDS	1389.14	1221.96	0.603	1.12
	pH	0.258	0.258	0.684	0.998
	EC	2190.09	0.0142	0.631	1.112
	SAR	2.372	0.0137	0.616	1.004
Circular	TH	431.9	398.6	0.689	1.08
	TDS	1322	1183.8	0.654	1.10
	pH	0.248	0.25	0.644	0.987
	EC	2133.84	0.01427	0.584	1.1132
	SAR	2.3194	0.0139	0.610	1.0392
Exponential	TH	444.64	413.37	0.701	1.07
	TDS	1384.24	1155.42	0.543	1.196
	pH	0.259	0.2581	0.584	1.002
	EC	2188.5	0.01283	0.592	1.1385
	SAR	2.3668	0.01343	0.583	0.9839
Gaussian	TH	461.59	403.42	0.603	1.13
	TDS	1433.19	1185.85	0.579	1.196
	pH	0.259	0.258	0.554	1.002
	EC	2284.31	0.0189	0.601	1.1946
	SAR	2.5307	0.0195	0.592	1.1316

Table 5. Cross-validation results of Ordinary CoKriging technique

Model	Parameter	Root Mean Square	Average Standard Error	R	Root Mean Square Standardized
Spherical	TH	299.6	354.3	0.742	0.750
	TDS	1087.3	924.19	0.726	0.928
	pH	0.2481	0.2498	0.700	0.983
	EC	1641.09	-0.0014	0.751	1.004
	SAR	1.529	0.0577	0.721	0.8178
Circular	TH	363.29	446.5	0.750	0.704
	TDS	1100.12	1004.8	0.731	0.874
	pH	0.2488	0.250	0.698	0.987
	EC	1691.73	0.02472	0.762	0.887
	SAR	1.6307	0.0824	0.689	0.730
Exponential	TH	159.96	170.4	0.621	1.12
	TDS	1184.5	390.05	0.564	8.68
	pH	0.2394	0.247	0.621	0.938
	EC	1554.59	-0.8759	0.742	6.7061
	SAR	2.2068	-0.831	0.723	6.615
Gaussian	TH	420.42	407.9	0.590	1.01
	TDS	1282.28	1093.94	0.568	1.162
	pH	0.2508	0.250	0.601	0.998
	EC	1932.51	-0.029	0.701	0.9971
	SAR	2.0502	0.0601	0.712	0.8151

Table 6. Cross-validation results of deterministic techniques

Model	Parameter	Root Mean Square	R
RBF	TH	467.6	.0568
	TDS	1440.8	0.587
	pH	0.250	0.702
	EC	2305.29	0.625
	SAR	2.5069	0.628
Circular	TH	510.5	0.502
	TDS	1558.2	0.540
	pH	0.272	0.629
	EC	2510.35	0.512
	SAR	2.6276	0.562

Water quality parameters results demonstrated that hardness of water in the east of basin was observed to be more than maximum permissible classification of the WHO (1984), i.e. 400 mg L^{-1} (Fig. 2). The TDS values of the study area were more than 1000 mg L^{-1}, and below the drinking water standard (1000 mg L^{-1}). The high rate of TDS can be related to pollution through discharge of sewage in waste pits in the east of study region, however, most of the TDS values were higher than the normal water quality (Fig. 3).

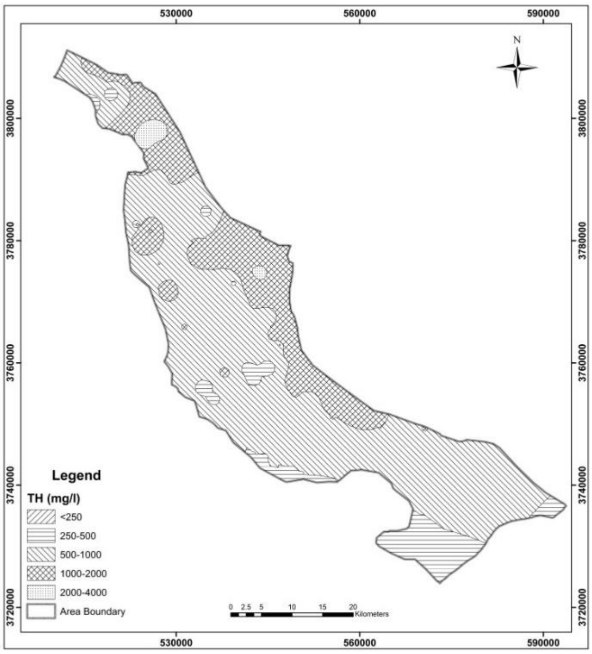

Fig. 2. Spatial distribution map of TH of Kashan plain

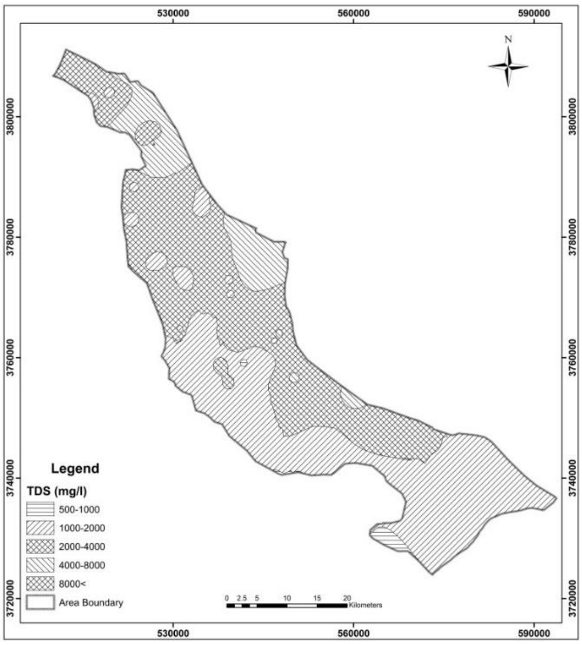

Fig. 3. Spatial distribution map of TDS of Kashan plain

The results showed that most of pH values of the case study were alkaline (Fig. 4). According to the WHO classification and standard, all the pH values were suitable for livestock and irrigation.

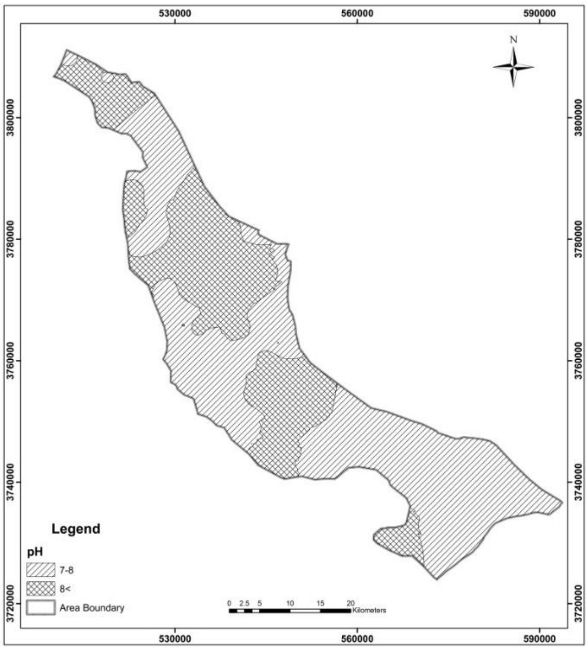

Fig. 4. Spatial distribution map of pH of Kashan plain

The EC values in the Kashan plain were totally different from north to south and from east to west (Fig. 5). According to the results, the electrical conductivity of groundwater varies between 340 µS cm^{-1} in Abuzeidabad and 22280 µS cm^{-1} in Yazdel. Based on the WHO classification, it was highly suitable for drinking purposes (1.500 µS cm^{-1}) in the south of the study region. Generally, EC increase is recorded from south to north and from west to east possibly due to reduction water table. These results were supported by Jafari and Bakhshandehmehr (2014).

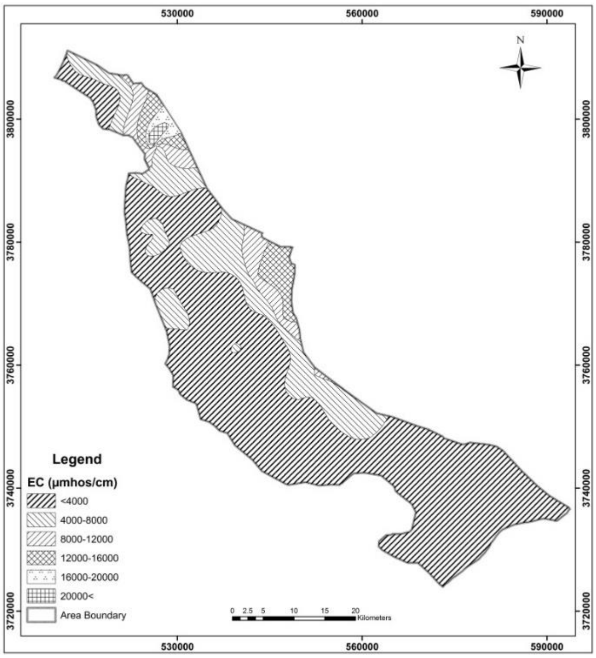

Fig. 5. Spatial distribution map of EC of Kashan plain

The Wilcox diagram based on SAR is also divided into four categories. The SAR of the case study is classified into two classes (S_1 and S_2, Fig. 6); therefore, in the study area, the SAR values were suitable. The results showed that the amount of electrical conductivity was less than the ratio of sodium absorption of groundwater in mountainous and flat areas.

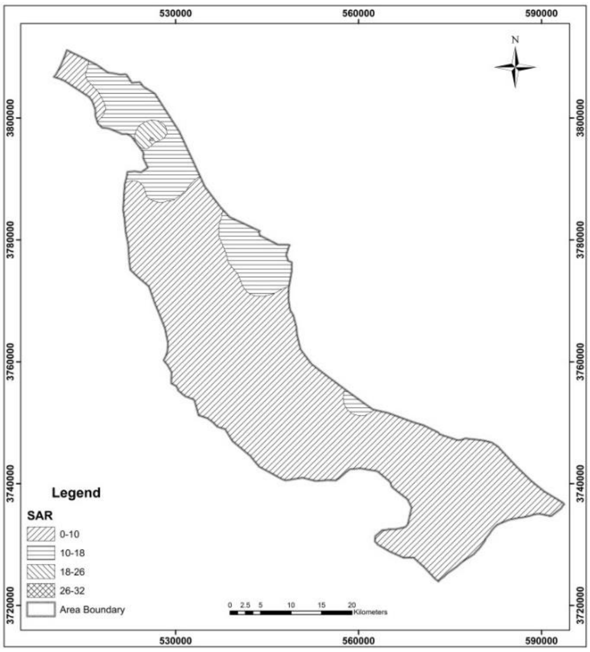

Fig. 6. Spatial distribution map of SAR of Kashan plain

Based on the results in Table 7, approximately 22 percent of the groundwater had good quality in the area. These groundwater resources could be found in the south and western parts of the region (Fig. 7). Suitable ground water for irrigation purposes (approximately 65% of the groundwater resources) were in the highlands of the west and south of the region.

Table 7. Groundwater quality classification using Wilcox method of Kashan plain

Water quality	Class	Area (ha)	Area percentage (%)
Good	C_2S_1	38023	21.84
Medium Quality	C_3S_1	73088	41.98
Medium Quality	C_3S_2	72	0.04
Non Suitable	C_4S_1	29154	16.75
Non Suitable	C_4S_2	28470	16.35
Non Suitable	C_5S_1	5293	3.04

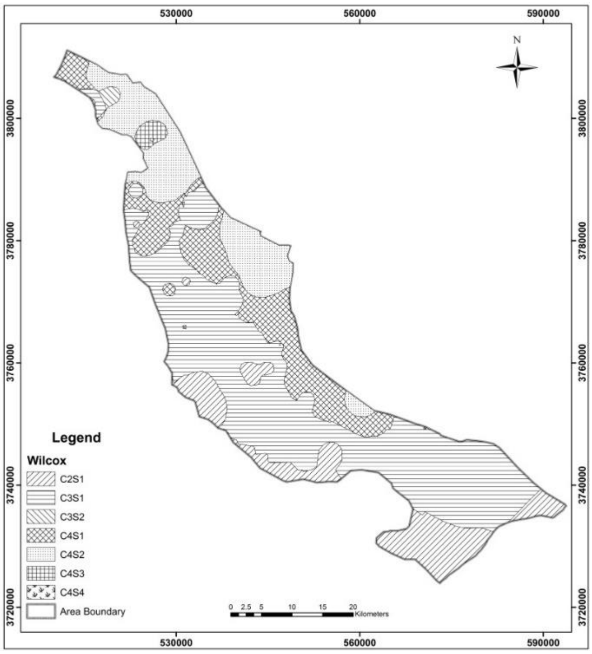

Fig. 7. Spatial distribution of water quality using Wilcox diagram of Kashan plain

Studies have indicated that decrease of water table in the south of the study area is more than that in the north of the plain. Since agricultural lands are located in the south of the plain and water consumption in these areas had the highest volume, then the greatest decrease of water table was observed in these areas. In similar studies (Rahmani *et al*., 2009; Jafari and Bakhshandehmehr, 2014), it was also noted that excessive use of groundwater resources was one of the most important factors in the decline of water table.

4. Conclusion

Groundwater is an essential water source in the Kashan plain, Iran. Almost more than 80% of the Kashan's water usage has been supplied from groundwater wells. The primary goal of the current research was to map and evaluate the groundwater quality in the study area. In this research, groundwater quality analysis was conducted on the data received for 72 observation wells in the Kashan plain applying deterministic and geostatistics techniques.

The spatial distribution of five groundwater quality parameters such as water quality parameters, including Electrical Conductivity, Sodium Adsorption Ratio, Total Hardness, Total Dissolved Solids and pH, was carried out through deterministic and geostatistical techniques. According to the spatial distribution maps of various water quality parameters, (Fig. 3) the south and southwest of the plain have the optimum groundwater quality, and generally, the groundwater quality decreases from the southwest to northeast of the plain.

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