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Case Record of Multivariate Statistical Analysis in the Groundwater Study of the Western Part of Iran (The Zagros Mountains)

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ABSTRACT

On large territories defining a site of groundwater with a similar chemical composition using a wide range of chemical elements and compounds (10 or more) is a rather complicated task. We have suggested the new way based on applying cluster analysis. Using this method gives an opportunity to find groundwater with a similar chemical composition in different areas and underground reservoirs. This method has been tested in the study of the chemical composition of the groundwater of the Shiraz and the Khorramabad intermountain basins, Iran.

KEY WORDS: Iran, the Shiraz and the Khorramabad intermountain basins, area, groundwater, similar chemical composition, cluster analysis.

INTRODUCTION

Problem statement

The groundwater of the Shiraz intermountain basin is widely used for water supply, industrial needs, agricultural irrigation and other purposes. The groundwater of the basin in the drainage zone has mineralization of up to 1 g/dm^3, and in the discharge zone mineralization is reasonably increased which is explained by continental salinity and man-made pollution (fertilizing, chemical industry waste and mine drainage). The groundwater has sulfate-chloride calcium-magnesium composition which corresponds to the drinking water standards. The type of water in the north-west and south-east of the basin is hydrocarbonate calcium-magnesium. The groundwater also contains heavy metals.

At the moment a wider usage of the groundwater of the Khorramabad intermountain basin is being planned as well.

Analysis of the published works and defining the unsolved problems:

The geological structure and hydrogeological conditions of the Khorramabad intermountain basin were explored by the following Irani companies: (*Sangab*, 2010, 1980); (*Abkav*, 1970); (*NKRC*, 1995, 1997). The companies mentioned above have compiled geological and hydrogeological maps, studied the chemical composition of the underground reservoir, and defined the hydrogeological parameters of the underground reservoir. A major contribution to the study of the hydrogeological conditions of the Khorramabad intermountain basin has been made by the department of hydrogeology of the Moscow State University (Shestakov V.M.)

The companies *Sangab* (2010), *Abkav* (1980), *NKRC* (1991, 1996, 1997), *Mahabkods* (1975) and *Parab* (1993, 1997) have explored the geological structure and hydrogeological conditions, as well as the chemical composition and hydrogeological parameters of the groundwater of the Shiraz intermountain basin. The results of theses surveys were reflected in the following published papers: James and Winds, Stöklin, Wells, Kent, Setudenia and Alavi. No definition of the groundwater sites with a similar chemical composition in the Shiraz and the Khorramabad intermountain basins has been realized. We have suggested a new way of defining groundwater sites with a similar chemical composition based on applying cluster analysis. The issue of applying cluster analysis in the study of the chemical composition of groundwater was covered in the works of Davis J.C., Iskenrog K.G., Reshetov I.K., Chomko D.F., Chomko F.V., Seifeldin G.Kh., Taranov V.G. et al.

Using this analysis makes it possible to find and delineate groundwater with a similar chemical composition in different regions and sites. This will not only allow to define similarities and differences in recharge and discharge, processes affecting formation of the chemical composition of groundwater, their possible contamination and exhaustion, but also to elaborate out measures in prevention of the latter. There is no literature about applying cluster analysis to define similarities in the chemical composition of the groundwater in Iran.

Survey objective

At present with the aim of defining similarity in the chemical composition of groundwater in different regions and underground reservoirs various analytical methods and mathematical modeling are used. But these

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methods use datasets with a rather small amount of data. Nowadays methods of multivariate statistical analysis are being increasingly used for this aim.

These methods are ones of the most effective ways of defining patterns contained in large amounts of data, since in hydrogeology there tends to be no possibility of direct observation and measuring. The pattern can only be analyzed on the basis of final results of occurrence of the processes reflected in the values of different characteristics, for instance the chemical composition of water.

The chemical composition of groundwater is the end-product of the effect of a complex of natural and technology-related processes (conditions of recharge and discharge, ion exchange, industrial pollution etc). The impact of these processes affects the interconnected alterations in the content of chemical components and the type of linkage between them. However, this linkage of the components of the groundwater being observed does not remain in pure form. The correlation dependence between the variable values observed is actually the final result of the effect of the complex of these processes. Under the conditions of natural flow any underground reservoir is a balanced system.

It is suggested to use the Euclidean distance in the n-dimensional space as the criterion of similarity estimation of the chemical composition of different water. This value is calculated for any quantity of hydrochemical components. Cluster analysis is realized according to the agglomerative hierarchical procedure with dendrogram creating (one-dimensional graph) depicting the linkage between the objects. The essence of agglomerative clustering process consists in calculating the function of distance between all the pairs of objects and linkage, at each step, of the pair of objects that demonstrates the minimal Euclidean distance. This allows to distinguish several clusters in the Euclidean distance structure that contain water with a similar chemical composition, i.e. a combination of water samples similar in the chemical composition.

Let the multitude $I = I_1, I_2, \ldots, I_n$ represent the data of chemical composition of the groundwater from wells and springs of different regions of the Shiraz and the Khorramabad intermontane plains showing *n* objects belonging to a population $_I$. Suppose each object has a multitude of key figures being observed $C = (C_1, C_2, \ldots, C_p)^T$. The figures being observed are quantitative data called measurements. They characterize chemical proprieties in each analysis *I*. The result of measuring of the *i*-th characteristic of the object I_j will be represented by the symbol $X_{i,j}$, and the vector $X_j = x_{i,j}$ of the dimension $P=1$ corresponds to every measurement series for the *j*-th individual. Thus for a multitude of individuals *I* there exists a multitude of measurement vectors $X = X_1, X_2, \ldots, X_n$, that describe the multitude *I*.

The Euclidean distance in the n-dimensional space is defined according to the following formula:

$$\boxed{D_{i,j} = \sqrt{\sum_{K=1}^{N}\left(X_{K,i}^{S} - X_{K,j}^{S}\right)^{2}}} \qquad (1)$$

where:

$D_{i,j}$ – Euclidean distance;

N – quantity of characteristics (the quantity of definite chemical elements and compounds in the analysis of one or another object);

$\boxed{X_{k,i}^{S}}$ – standardized value of the *K*-th characteristic of the *i*-th object;

$\boxed{X_{k,j}^{S}}$ – standardized value of the *K*-th characteristic of the *j*- th object;

The standardized value of the *K*-th characteristic of the *i*-th object is defined according to the following formula:

$$\boxed{X_{K,i}^{S} = \frac{X_{K,i} - \overline{X_K}}{\sigma_K}}, \qquad (2)$$

where:

$X_{K,i}$ – value of the *K*-th characteristic of the *i*-th object;

$\boxed{X}_K$ – average value of the *K*-th characteristic in *N* objects;

$_K$ – standard deviation of the *K*-th characteristic in *N* objects.

The standardized value of the *K*-th characteristic of the j-th object is defined according to the following formula:

$$\boxed{X_{K,j}^{S} = \frac{X_{K,j} - X_K}{\sigma_K}}, \qquad (3)$$

where:

$X_{K,j}$ – value of the *K*-th characteristic of the *j*-th object;

$\boxed{X}_K$ – average value of the *K*-th characteristic in *N* objects;
$_K$ – standard deviation of the *K*-th characteristic in *N* objects.

Creating an accurate dendrogram requires standardization (normalization) of the original data. Standardization is a transition to some uniform description for all the measurements (characteristics), introduction of a new standard unit of measuring allowing formal comparison of objects. The program realizes a standard normalization of measurements in standard deviations according to the formula:

$$\boxed{Z = \frac{(X - \overline{X})}{\sigma}}, \qquad (4)$$

where: $\boxed{\overline{X}, \sigma}$ – average and standard deviation of *X* correspondingly.

The standard unit of measurement *Z* is calculated for any quantity of chemical elements. The influence of a separate component on the key figure does not depend on its absolute value but on its relative difference in the component in different objects which is evaluated according to its contribution to the weight index. The weight of the component is defined as the ratio of the average value of this component to the average value of all the components calculated separately for each object.

Realization of this method implies using the data of chemical analyses of the groundwater located in different places of the Shiraz and the Khorramabad intermountain basins. Defining the chemical composition of the groundwater was implemented in an accredited laboratory in Tehran for the uniform period of time (July).

In the process of calculation the following characteristics of the chemical composition of the groundwater were considered: Ca, Mg, Na, HCO_3, SO_4, Cl, pH, mineralization, Cd, Co, Ba, Cu, Mo, Ni, Pb, Zn and Fe. Thus each 61-th chemical analysis of the groundwater is interpreted as a point in the 17-dimension space. The chemical composition of the groundwater of the Shiraz and the Khorramabad intermountain basins is reflected in the Tables 1 and 2.

The analysis results of the chemical composition of the groundwater, given in the table, need to be recorded as a matrix and cluster analysis needs to be implemented. The first matrix (the Shiraz valley) contains chemical analyses of the groundwater samples taken from 23 wells and 6 springs, and the second one (the Khorramabad valley) – from 14 wells and 18 springs. They are characterized by 17 chemical elements and chemical compounds.

Table1. The chemical composition of groundwater Shiraz intermountain basin (dm 3)

The source type	Cd	Co	Ba	Cu	Mo	Ni	Pb	Zn	Fe	PH	Cl	HCO3	SO4)	Ca	Mg	Na	Tds	ECµmo
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Pirbona. w	0.007	0,00001	0.001	0.014	0,00001	0.01	0,00001	0.393	0.032	8,3	43	165	202	68	50	28	530	740
Pol-berenji.spr	0.007	0,00001	0.028	0.015	0.017	0.004	0,00001	0.425	0.214	8,3	391	195	79	72	28	201	940	1670
Babahaji. w	0.004	0.005	0,00001	0.003	0.008	0.03	0.001	0.145	0.027	8,3	53	185	231	78	50	41	580	937
Pol-fasa.w	0.008	0,00001	0.002	0.019	0,00001	0.02	0,00001	0.398	0.038	8,2	58	201	210	74	51	38	605	904
Barmedade. spr	0.004	0.011	0.003	0.014	0,00001	0.01	0,00001	0.388	0.039	7,8	56	238	189	72	54	36	617	873
Kaftarak .w	0.005	0.013	0.005	0.005	0.005	0.015	0.023	0.039	0.038	8,2	57	256	192	74	54	33	630	869
Barmedelak. spr	0.008	0.015	0.004	0.006	0.006	0.014	0.026	0.04	0.037	7,8	57	305	154	82	55	33	640	869
Barmetaer. spr	0.008	0.015	0.004	0.006	0.006	0.014	0.026	0.04	0.037	7,5	184,9	305	205	104	67	378	1571	2290
Barmeshur. w	0.006	0.01	0.001	0.01	0.014	0.016	0.007	0.244	0.162	7,9	185	305	230	117	77	548	1974	3050
Barmekhan. spr	0.006	0.03	0.015	0.377	0.051	0.044	0.046	0.122	1.472	8,3	1018	244	255	120	80	718	2380	3810
Brmebabuna k.spr	0.002	0.01	0.014	0.012	0.007	0.004	0.023	0.04	0.12	8,3	1206	244	264	160	61	856	2700	4346
Soltanabad. w	0.002	0.012	0.035	0.006	0.014	0.01	0.016	0.018	0.096	8,2	85	194	283	94	64	58	760	1132

Sadi.w	Ghasrgushe .w	Mohammad. w	Mansurabad. w	Shams.w	Khabir.w	Moinabad. w	Khatunak. w	Pir-mohammad .w	Mahmudabad .w	Ghachi .w	Jarestan. w	Kruni. w	Shapur. w
0,00001	0.007	0.004	0.01	0.002	0.006	0.006	0.006	0.007	0.005	0.004	0.007	0.006	0.002
0.01	0.027	0.036	0.014	0.003	0.004	0.005	0.009	0,00001	0.015	0.018	0.02	0.01	0.015
0,00001	0.043	0.037	0.004	0.018	0.016	0,00001	0.024	0.029	0.023	0.004	0.006	0.025	0.03
0.011	0.039	0.036	0.018	0.035	0.011	0.013	0.017	0.016	0.021	0.015	0.009	0.024	0.017
0.003	0.012	0.025	0.032	0.008	0,00001	0,00001	0.017	0.018	0.056	0.012	0.005	0.059	0.048
0.019	0.036	0.049	0.019	0.004	0.021	0,00001	0.082	0.005	0.085	0.039	0.009	0.087	0.004
0.02	0.019	0.045	0.042	0.016	0.024	0.039	0.027	0,00001	0.038	0.032	0.002	0.041	0.23
0.173	0.09	0.092	0.065	0.063	0.147	0.13	0.025	0.429	0.305	0.051	0.196	0.315	0.057
0.295	0.128	0.264	0.219	0.046	0.002	0.054	0.047	0.218	1.384	0.099	0.203	1.391	0.298
7,4	7,8	7,6	7,4	7,3	7,6	7,3	7,88	7,9	8,2	7,4	8	8,5	8
142	333	25	21	25	18	21	184,9	185	64	64	71	92	85
232	226	226	226	299	232	214	225,52	225,5	220	220	195	207	180
744	1047	73	67	106	62	59	107	154	250	231	264	288	283
221	349	52	56	84	60	46	58	71	94	98	90	118	98
61	27	30	27	34	28	33	36	39	47	47	52	58	43
171	213	19	13	21	13	10	17	25	40	40	45	57	50
1327	2130	384	367	501	376	351	435	518	677	665	686	700	665
2280	2950	545	537	695	520	486	509	703	918	936	1000	1170	1035

Abkhan.w	0,00001	0.017	0.038	0.039	0.095	0.038	0.023	0.146	1.338	8,1	301	275	288	94	75	201	1190	1820
Aliabad.w	0.006	0.02	0.005	0.019	0.016	0.04	0.036	0.065	0.01	7,3	50	281	180	80	49	32	624	854
Bahram.w	0,00001	0.021	0.013	0.027	0.018	0,00001	0.027	0.073	0.047	8	234	238	317	92	90	133	1715	2500

Table2. The chemical composition of groundwater Horramabadskoy intermountain basin (dm 3)

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Rashidi-darai.w	0,0005	0,004	0,015	0,003	0,00001	0,0004	0,0008	0,005	0,048	7,28	80	300	60	230	170	13	384	600
Malekshahi.w	0,00008	0,0008	0,074	0,048	0,00001	0,001	0,005	0,00001	0,11	7,02	30	510	57	350	240	6	441	690
Naservand.w	0,00009	0,001	0,066	0,004	0,0004	0,0013	0,0005	0,007	0,00001	7,41	60	400	157	280	220	108	364	570
Dehbagher.w	0,00005	0,001	0,01	0,002	0,004	0,0016	0,0008	0,0009	0,059	7,21	130	570	3	390	280	29	643	990
Borjali.spr	0,0001	0,001	0,192	0,001	0,001	0,003	0,0002	0,014	0,04	7,41	20	320	20	180	200	1	236	370
Sorkhedeh.spr	0,00008	0,003	0,2	0,001	0,001	0,003	0,0001	0,008	0,056	7,83	330	390	178	340	240	290	650	1000
Robatnamaki.w	0,00009	0,001	0,17	0,001	0,001	0,003	0,0005	0,004	0,021	7,71	160	460	55	350	300	20	507	780
Kelmekhub.spr	0,0002	0,002	0,21	0,003	0,00002	0,005	0,001	0,0008	0,11	7,4	80	530	143	360	250	108	409	640
Cheshmebid.spr	0,0001	0,002	0,23	0,003	0,0005	0,005	0,003	0,019	0,04	7,38	40	350	14	390	10	4	188	450
Sarabe-sgha.spr	0,0002	0,003	0,09	0,002	0,00001	0,0034	0,0007	0,004	0,07	7,5	40	530	92	430	200	26	416	650

Chamgharg .w	Changai .spr	Sarnamak.w	Chogharushi .w	Ali-abad.w	Kahriz.spr	Sarabe-yas.spr	Giluran.w	Navekesh. spr	Cheshme-sorkhe.spr	Sabur.w	Cheshme-cheragh.spr	Ghale-joghd.spr
0,0001	0,00009	0,0001	0,00001	0,0001	0,00008	0,00007	0,00005	0,00001	0,00008	0,00009	0,0002	9,0001
0,0008	0,008	0,002	0,0013	0,0013	0,003	0,004	0,003	0,002	0,0014	0,008	0,001	0,001
0,08	0,08	0,19	0,07	0,01	0,015	0,01	0,015	0,08	0,01	0,08	0,2	0,08
0,04	0,04	0,003	0,005	0,02	0,006	0,005	0,003	0,005	0,002	0,046	0,002	0,0009
3E-06	0,00003	0,0003	0,0005	0,00004	0,00001	0,00002	0,00001	0,0006	0,003	0,00001	0,00002	0,0009
0,001	0,001	0,003	0,002	0,004	0,004	0,0004	0,0005	0,002	0,0017	0,002	0,002	0,003
0,00005	0,04	0,0006	0,006	0,00001	0,0007	0,00007	0,0008	0,006	0,0009	0,005	0,004	0,0002
0,05	0,05	0,015	0,008	0,007	0,004	0,005	0,005	0,008	0,0009	0,005	0,004	0,006
0,09	0,09	0,04	0,1	0,098	0,049	0,04	0,04	0,1	0,06	0,9	0,001	0,016
7,18	7,23	7,18	7,16	7,52	7,64	7,34	7,26	7,18	7,97	7,54	7,23	7,32
160	80	160	70	50	30	70	120	30	70	40	70	20
600	470	600	690	340	270	490	490	390	330	380	430	360
65	9	65	64	142	98	127	5	24	71	52	11	5
450	380	450	210	290	250	370	390	360	300	340	330	330
360	160	360	510	160	8	210	200	80	110	110	110	50
16	16	16	95	73	56	90	24	3	39	18	65	6
669	468	669	494	313	224	435	624	326	275	294	371	294
1030	720	1030	760	490	350	680	960	510	430	460	580	460

Balilvand .w	Darband.w	Sarabe-ghurchi.spr	Cheshme-tala.spr	Kiv.spr	Gerdabsangi .spr	Gushe.spr	Dore.spr	Charkal.w
0,004	0,002	0,0002	0,00002	0,00002	0,0002	0,00008	0,00005	0,00008
0,004	0,001	0,003	0,002	0,001	0,001	0,0007	0,001	0,002
0,015	0,06	0,08	0,2	0,1	0,1	0,07	0,08	0,1
0,003	0,007	0,05	0,04	0,002	0,002	0,04	0,006	0,001
0,00005	0,0001	0,00001	0,00001	0,00005	0,00007	0,00001	0,0008	0,001
0,0004	0,002	0,0035	0,003	0,003	0,004	0,001	0,002	0,003
0,093	0,0008	0,005	0,004	0,001	0,0001	0,004	0,00007	0,00001
0,006	0,0006	0,005	0,003	0,0007	0,0008	0,004	0,009	0,008
0,05	0,004	0,09	0,053	0,098	0,09	0,09	0,15	0,05
7,4	7,54	7,41	8,16	7,56	7,38	7,66	7,02	7,47
60	70	60	60	20	40	10	30	285
530	370	400	450	380	350	290	610	810
143	106	157	9	1	14	90	57	193
360	320	280	350	290	390	350	350	260
250	170	220	150	8	10	40	240	440
108	63	108	9	2	4	1	96	600
409	342	364	345	294	288	236	441	838
640	523	570	540	4650	450	370	690	1270

Principal results of cluster analysis

Cluster analysis is implemented according to the program CLUSTER elaborated by the department of hydrogeology of V.N.Karazin Kharkiv National University and is implemented according to the “complete-linkage” method. Cluster analysis of the chemical composition of the water is implemented according to the “complete linkage” method. The “furthest neighbor” and the “nearest neighbor” methods demonstrate similar results.

The Shiraz intermountain basin

Based on the results of cluster analysis of the first matrix the plot of linkage distance across steps (Fig. 1) and the dendrogram (Fig. 2) have been created.

Fig. 1 shows that the linkage of all the chemical compositions occurred in 29 steps. The minimal linkage distance (Euclidean distance) at the first step equals 0.000 and the maximal one – 4750.28 at the last 29th step. The basic amount of chemical analyses (21) linked at the distance from 0.000 to 375.012. This, in our opinion, proves uniformity of the chemical composition of the groundwater samples obtained in the Shiraz basin.

The dendrogram (Fig. 2) shows that in the result of cluster analysis all the chemical analyses of the groundwater from the wells and springs, located in different parts of the Shiraz intermountain basin, are divided into 5 clusters (groups) that, in their turn, form smaller subgroups

The first cluster consists of 2 subclusters (subgroups).

The *first subcluster* unites analyses of the chemical composition of the groundwater taken from 3 wells (Pirbona, Pirmokhamad, Shams) from different sites of the Shiraz intermountain basin. Linkage of these analyses occurred on rather small Euclidean distances (from 180.185 to 187.453).

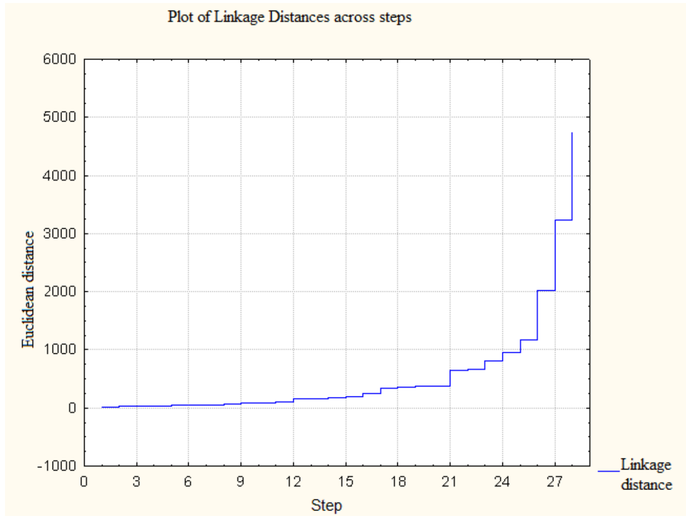

Fig. 1. Diagram of Linkage Distances across steps (the Shiraz basins)

The *2nd subcluster* unites analyses of the chemical composition of the groundwater taken from 5 wells (Khatunak, Moniabad, Khabir, Mansurabad, Mohammad). Linkage of these analyses occurred on rather small Euclidean distances (from 0.0 to 184.673). Linkage of these two subclusters in the first cluster occurred at the Euclidean distance of 370.043. The analysis of the Euclidean distances, where linkage of chemical analyses of groundwater of the Shiraz basin occurred in the first cluster, proves their significant similarity.

All the wells of the first subcluster are located in the Karabakh basin. The three wells of the second cluster are located at the foot of mount Darak and one of them (Mohammad) is in the valley of the river Khoshkrud which flows in the Shiraz basin. Thus we have singled out 3 sites of groundwater with a rather similar chemical composition that belong to the first cluster. (Fig. 3). The *second cluster* unites chemical compositions of the groundwater samples taken from 10 wells and 2 springs on different sites of the Shiraz basin.

The second cluster consists of three subclusters (subgroups) (Fig. 2).

The *first subcluster* unites groundwater samples from the wells of Babahaji, Polefasa, Gachi, Mahmudabad, Shams, Jarestan. Linkage of these chemical compositions occurred at rather small Euclidean distances (from 0.000 to 120.717). The *second subcluster* unites groundwater samples from the wells of Kaftarak, Aliabad and the springs Barmedade and Barmedelak. Linkage of these chemical compositions occurred at rather small Euclidean distances (from 0.000 to 50.01). The *third subcluster* unites groundwater samples from the wells of Soltanabad, Kruni. Linkage of these chemical compositions occurred at rather small Euclidean distances.

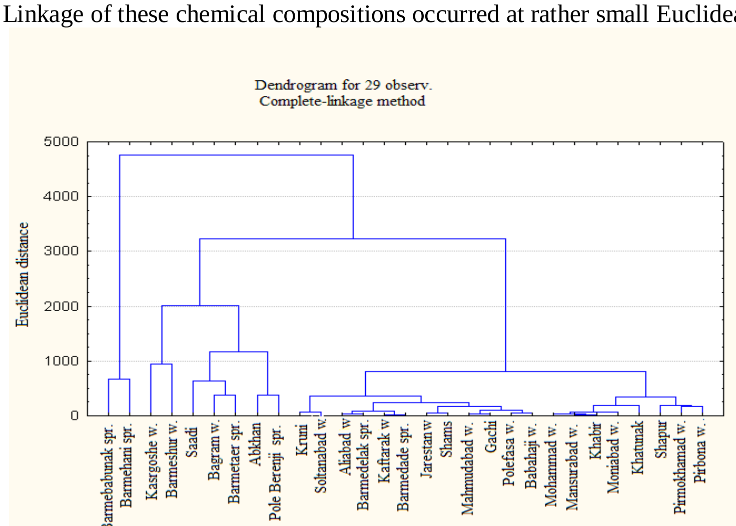

Fig. 2. Plot of linkage of 29 analyses of the chemical composition of the groundwater (17 chemical elements and compounds).

The groundwater belonging to the second cluster is located on two sites with the same chemical composition of the groundwater. The first site is in the valley of the river Babahaji at the foot of mount Soltanabad, and the second site is singled out at the foot of mount Kaftarak in the valley of the river Khoshkrud. Thus we have defined two sites of groundwater with a significantly similar chemical composition that belong to the second cluster (Fig. 3).

The third cluster consists of two subclusters (Fig. 2). In the *first subcluster* linkage of the chemical compositions of the groundwater from the well Abkhan and the spring Pole Berenji occurred at the Euclidean distance of 402.541.

The *second subcluster* contains samples of the groundwater from the spring Barmetaer and the wells Abkhan and Saadi that linked at the distance of 754.064. The first and the second subclusters linked at the Euclidean distance of 1206.754.

The groundwater belonging to the third cluster is located on three sites with a similar chemical composition of groundwater. The first site is in the valley of the river Babahaji at the foot of mount Soltanabad, the second site is defined at the foot of the Zagros mountains and on the third site at the foot of the mount Saadi there is one well Saadi.

The fourth cluster consists of chemical analyses of the groundwater from the wells Barmeshur and Kasrgoshe that linked at the Euclidean distance of 954.08 (Fig.2). The Barmeshur well is located in the valley of the river Polefasa not far from the lake Maharloo, and the Kasrgoshe well is on the north of the Shiraz basin between Mounts Saadi and Darah.

The third and the fourth clusters link in one cluster at the Euclidean distance of 2005.087 and link with the first two ones at the distance of 3236.512. This means that the chemical compositions of the groundwater forming this cluster differ greatly from the chemical composition of the water from the first cluster.

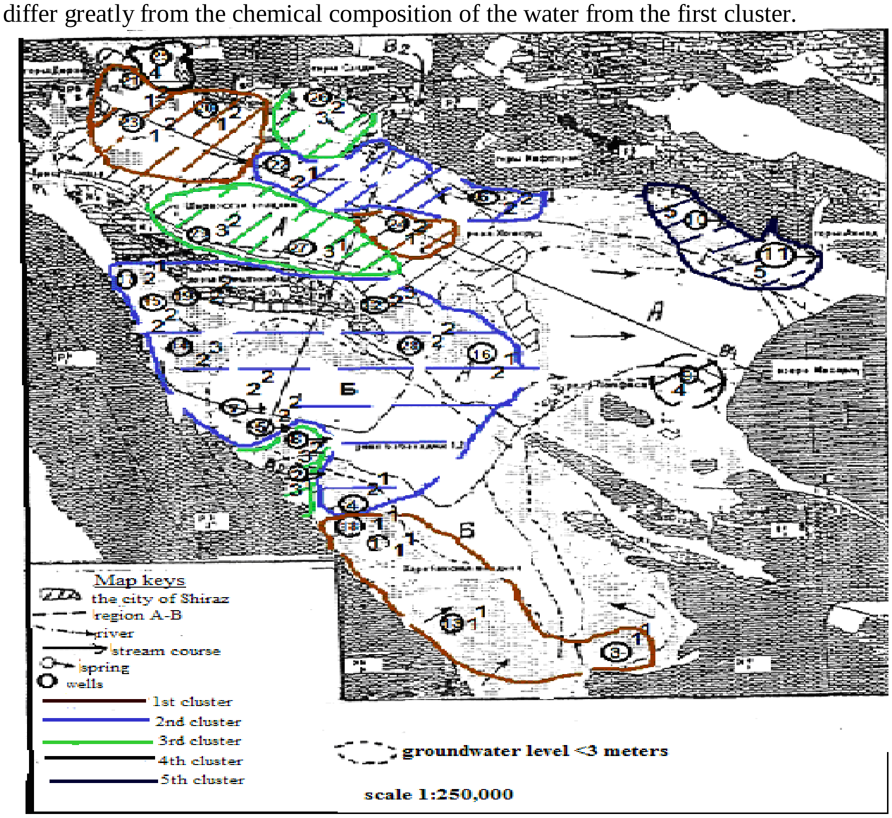

Fig. 3. Hydrogeological map of the Shiraz intermountain basin

The **fifth cluster** is formed by the chemical compositions of the samples from two springs Barmehani and Barmebabunak (Fig. 2) that are located at the foot of mounts Kaftarak and Akhmad. The fifth cluster links with the rest of the clusters at the distance of 4753.095. In our opinion the water of these two springs is of completely different nature.

The Khorramabad intermountain basin

Based on the results of cluster analysis of the second matrix the plot of linkage distances across steps (Fig. 4) and the dendrogram (Fig. 5) have been created.

Fig. 4 shows that linkage of all chemical analyses of the groundwater occurred in 32 steps. The minimal linkage distance (Euclidean distance) at the first step equals 0.000 and the maximal one – 4275.257 at the last 32nd step. The basic amount of analyses (28) linked at the distance from 0.000 to 495.264. This, in our opinion, proves uniformity of the chemical composition of the groundwater samples obtained in the Khorramabad basin.

The dendrogram (Fig. 5) shows that in the result of cluster analysis all the chemical analyses of groundwater from the wells and springs, located in different parts of the Khorramabad intermountain basin, are divided into 6 clusters (groups) that, in their turn, form smaller subgroups.

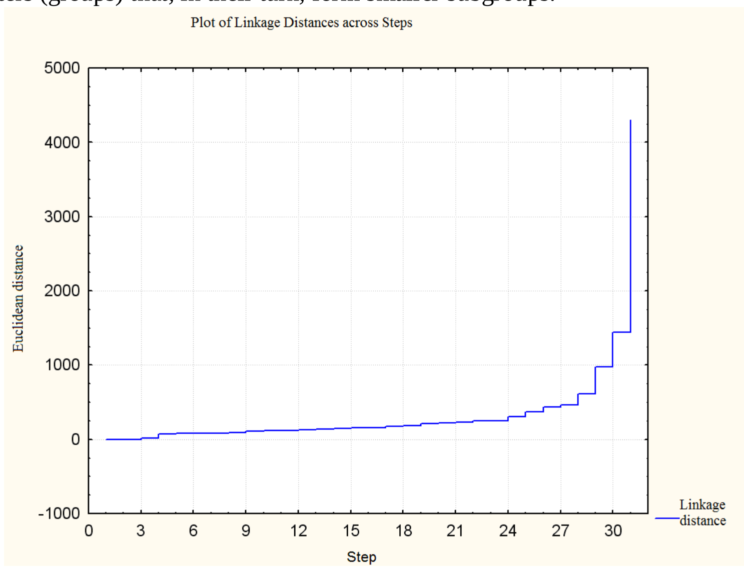

Fig. 4. Plot of Linkage Distances across steps (the Khorramabad intermountain basins)

The first cluster consists of 2 subclusters (subgroups).

The *first subcluster* unites analyses of the chemical composition of groundwater taken from 4 wells (Rashidi-Darani, Naservand, Aliabad, Darband) and one spring (Sarabe Gorchi) from different sites of the Khorramabad intermountain basin. Linkage of these analyses occurred on rather small Euclidean distances (from 0.000 to 129.373). The 2^{nd} *subcluster* unites analyses of the chemical composition of the groundwater taken from 2 springs Cheshmeh Cheragali and Cheshmeh Tala linked at the Euclidean distance of 102.36. These springs come from karst.

Linkage of these too subclusters in the first cluster occurred at the Euclidean distance of 239. 403. Analysis of the Euclidean distances, where linkage of the chemical analyses of the groundwater of the Khorramabad basin occurred in the first cluster, proves their significant similarity.

All the wells of the first subcluster are located in the south-west part of the Khorramabad basin. Only one spring Cheshme Cheragali is located in the northern part of the basin. Thus we have singled out 2 sites of groundwater with a rather similar chemical composition that belong to the first cluster. (Fig. 6).

The second cluster consists of two subclusters (subgroups) (Fig. 5).

The *first subcluster* unites chemical compositions of the groundwater samples from the springs of Borjali, Kahriz and Gushe that linked at the small Euclidean distance of 250.265. These springs are located in the western part of the basin. The *second subcluster* unites groundwater samples from the springs of Cheshme Bid, Qaleh Joghd, Gardabsangi, Navekesh, Cheshme Sorkhe and the well Sabur at small Euclidean distance of 241.712. Linkage of these too subclusters in the second cluster occurred at the Euclidean distance of 297.548. The analysis of the Euclidean distances, where linkage of the chemical analyses of the groundwater of the Khorramabad basin occurred in the second cluster, proves their significant similarity.

The springs Cheshme Bid, Qaleh Joghd and Gerdabsangi are located in the northern part of the basin, the springs Borjali, Navekesh and Kahriz – on the site in the western part of the basin and the springs Cheshme Sorkhe, Gerdabsangi and the well Sabur are located on the site in the southern part of the basin. Thus we have defined three sites of the groundwater with a significantly similar chemical composition that belong to the second cluster (Fig. 6).

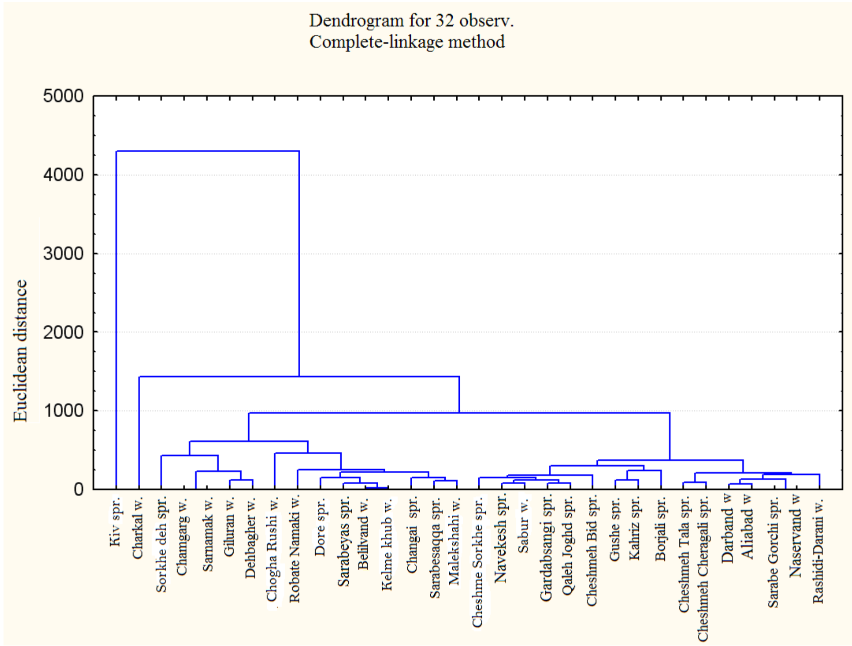

Fig. 5. Plot of linkage of 32 analyses of the chemical composition of the groundwater (17 chemical elements and compounds).

The third cluster consists of four subclusters (Fig. 5). In the *first subcluster* linkage of the chemical compositions of groundwater from the springs Sarabesaqqa, Changai and the well Meleh Shahi occurred at the small Euclidean distance of 131.431.

In the *second subcluster* the chemical cimpositions of the groundwater samples of three springs Kelmekhub, Sarabeyas, Darreh and the well Belilvand linked at the close Euclidean distance of 134.131.

These two subclusters linked at the Euclidean distance of 246.655. The chemical composition of the water sample from the well Robate Namaki (*the third subcluster*) joins them at the Euclidean distance of 250.065. The chemical composition of the water sample from the well Chogha Horushi (*the fourth* subcluster) joins them at the Euclidean distance of 489.785.

All the springs and wells of the third cluster are located on the site in the center of the Khorramabad intermountain basin and only the spring Doreh is located on the west of the basin. Thus we have defined two sites of groundwater with significantly similar chemical composition that belong to the third cluster (Fig. 6).

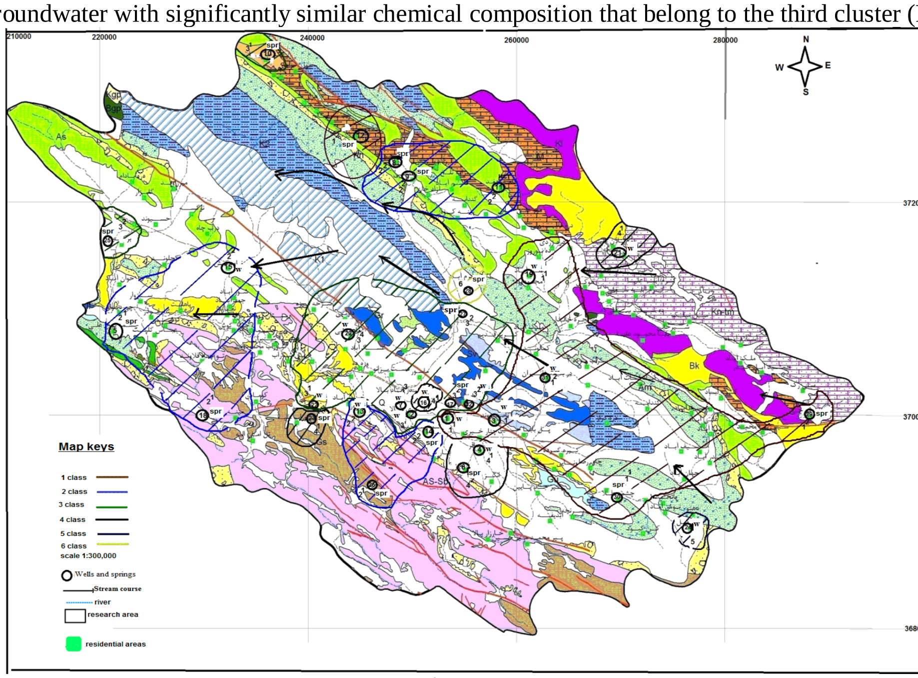

Fig. 6. Hydrogeological map of the Khorramabad intermountain basin

The fourth cluster consists of chemical analyses of the groundwater samples from three wells (Dehbagher, Giluran, Sarnamak) and the springs Chamgarg and Sorkhe de. Chemical analyses of the samples taken from the wells link at the Euclidean distance from 0.0 to 248.91. The chemical composition of the water sample from the spring joins them at the Euclidean distance of 416.72.

The third and the fourth clusters link at the Euclidean distance of 602.851 and link with the first two ones at the distance of 989.218.

The wells Dehbagher and the spring Sorkhe deh of this cluster are located on the site in the southern part of the basin, the well Sarnamak is located on the site that is in the east part, the spring Chamgarg is in the south-west part and the well Giluran is located in the central part of the Khorramabad basin and surrounded by the wells of the third cluster.

Thus we have defined four sites of groundwater with a significantly similar chemical composition that belong to the fourth cluster (Fig. 6).

The **fifth cluster** is formed by the chemical composition of the water samples from the well Charkal which is linked with the first four clusters at the significant Euclidean distance (1386.12). This well is located on the site in the south-east part of the Khorramabad basin.

The chemical composition of the water samples from the spring Kiv linked with the rest of the clusters at the significant Euclidean distance (4079.0). This spring is located in the central part of the basin. This proves that the chemical composition of the water from this spring is sharply different from the rest of the analyses and has a completely different nature.

CONCLUSIONS

- The analysis of the Euclidean distances where linkage of the chemical compositions of the groundwater of the first and the second clusters occurred, displays their significant similarity both in the Shiraz and the Khorramabad intermountain basins.
- The groundwater samples of the third cluster are slightly different from the samples of the first and the second clusters in the chemical composition. They are linked at a slightly larger distance than the one where linkage of the chemical analyses take place in the first and the second clusters.
- The chemical composition of the water of the fourth cluster are significantly different from chemical composition of the water included in the first three clusters.
- The fifth and the sixth clusters consist of three heterogeneous subclusters in which the chemical composition of the groundwater differ sharply both within the cluster and in comparison with the first four clusters. These groundwater are extremely contaminated and are in the discharge zone, where mineralization is much higher, which is explained by continental salinity and man-made pollution (fertilizing, chemical industry waste and mine drainage).
- On the basis of the analysis mentioned above it can be stated that cluster analysis allows:
- to define similarities and differences in the chemical composition of groundwater;
- in case any negative change has been discovered in the chemical composition of the groundwater in the Shiraz intermountain basin, it will be possible to judge about similar changes in the Khorramabad basin as well, and vice versa.
- to single out sites with a similar and different chemical composition of groundwater and delineate them;
- in the Shiraz intermountain basin we have singled out 3 groundwater sites with a rather close chemical composition that belong to the first cluster, two sites belonging to the second cluster, three sites belonging to the third cluster and one belonging to the fifth cluster;
- in the Khorramabad intermountain basin we have defined two groundwater sites with a rather close chemical composition belonging to the first cluster, three sites belonging to the second cluster, two sites belonging to the third cluster and one site for each of the fifth and the sixth sites;
- in our opinion under the condition of regular distribution of testing points (e.g., for groundwater survey), this method can be applied for zoning of the groundwater based on their chemical composition.

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