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Interpretation of Groundwater Chemistry by Factor Analysis Technique

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ABSTRACT. Factor analysis was applied to groundwater chemistry data of Khulais basin western Saudi Arabia to assess the usefulness of such method for interpreting the hydrochemical processes. Three factors were retained. The first two factors were adequate for describing the groundwater chemistry processes that have taken place in the area. These processes are: (1) groundwater mineralization due to evaporation, and mineral dissolution processes which are considered the most important, (2) processes of dissolution and precipitation of carbonate minerals. Factor analysis also provides a mechanism to identify the independent variables and help in delineation of highly mineralized zones already recognized in previous works.

Introduction

One of the major problems associated in groundwater chemistry evaluation is the availability of a large amount of base information concerning the groundwater quality particularly in regional studies. In general, the measurements, chemical and non-chemical carried out both in the field and laboratories, might reflect a number of variables which together make up the groundwater chemistry. Such variables obtained could cause rather complexity and confusion for investigation for giving a clear picture of the existing system under study (Usunoff and Guzman-Guzman 1989, Ashley and Lloyd 1978).

Several methods of data analysis have been devised to simplify interpretation and presentation such as Trilinear, Semilogarithmic, Durov diagrams, ... etc. (Lloyd and Heathcote 1985). The existing methods may provide some information. Nevertheless, these conventional techniques are generally limited to major constituent ions. They ignore many parameters which are otherwise important for hydrochemical studies. The limitation that coupled for using the traditional graphical methods are discussed by several authors (Sen and Al-Dakheel 1986, Lawrence and Upchurch 1982, Ashley and Lloyd 1978).

In view of the limitation of the existing methods and increasing number of chemical and physical variables measured in groundwater investigations, multivariate analysis comes into play as a rather essential tool for explaining groundwater chemistry conditions. Factor analysis (FA) is considered the most widely used in groundwater chemistry. The aim of using factor analysis is to simplify the quantitative description of a system by determining the minimum number of new variables necessary to reproduce various attributes of the data. These procedures reduce the original data matrix from one having n variables necessary to describe the N samples to a matrix with m factors ($m < n$) for each of the N samples (Davis 1973, Johnston 1980). Factor analysis (FA) has been successfully used in groundwater chemistry interpretation (Dawdy and Feth 1967, Dalton and Upchurch 1978, Usunoff and Guzman-Guzman 1989). Their work showed that FA can be used with the added advantage of being able to use number of variables describing the hydrochemical facies of groundwater and established map according to their factor classification results.

The purpose of this study is to demonstrate the usefulness of FA as a tool for identifying and explaining of the groundwater chemistry existing in Khulais basin in western province of Saudi Arabia from commonly collected groundwater chemistry data.

Study Area

The study was conducted in a 400 km^2 portion of Khulais basin, northeast of Jeddah city (Fig. 1). This area is considered the most important water supply to Jeddah. The climate is typically arid. The average rainfall is about 50 mm/annum. It is irregular and of torrential nature when it occurs. The study area has been the object of number of investigators (*e.g.*, Italoconsult 1976, AlNujaidi 1978, AlGamel and Sen 1983, Zaidi 1983 & 1984). As a result of these studies, several conclusions have been proposed to explain the hydrogeological, hydrochemical and geomorphological aspects that control the present conditions of the Khulais basin. In a recent study, Bazuhair *et al.* (1992) pointed out that the groundwater chemistry is spatially and temporally highly variable within the area. They showed that the salinity is rather high and it was attributed to the evaporation processes and recycle of irrigation water. The existing aquifers are mainly recharged through runoff events from three major wadis: Murawani, Abu Hulaifa and Ghiran (Fig. 1). The values of recharge from these events are unknown.

Geologic Setting

Few detailed studies concerning geological aspects are available. A brief description of the geological setup is found in Zaidi (1983 & 1984). In his report, he summarized four major geologic units in the area, from youngest to oldest (Fig. 2): (1) Quaternary superficial deposits that consist mainly of sand, siltstone, clay and wadi *gravel*; (2) Tertiary flows occurs as a series of basalt flows related to renewed rifting

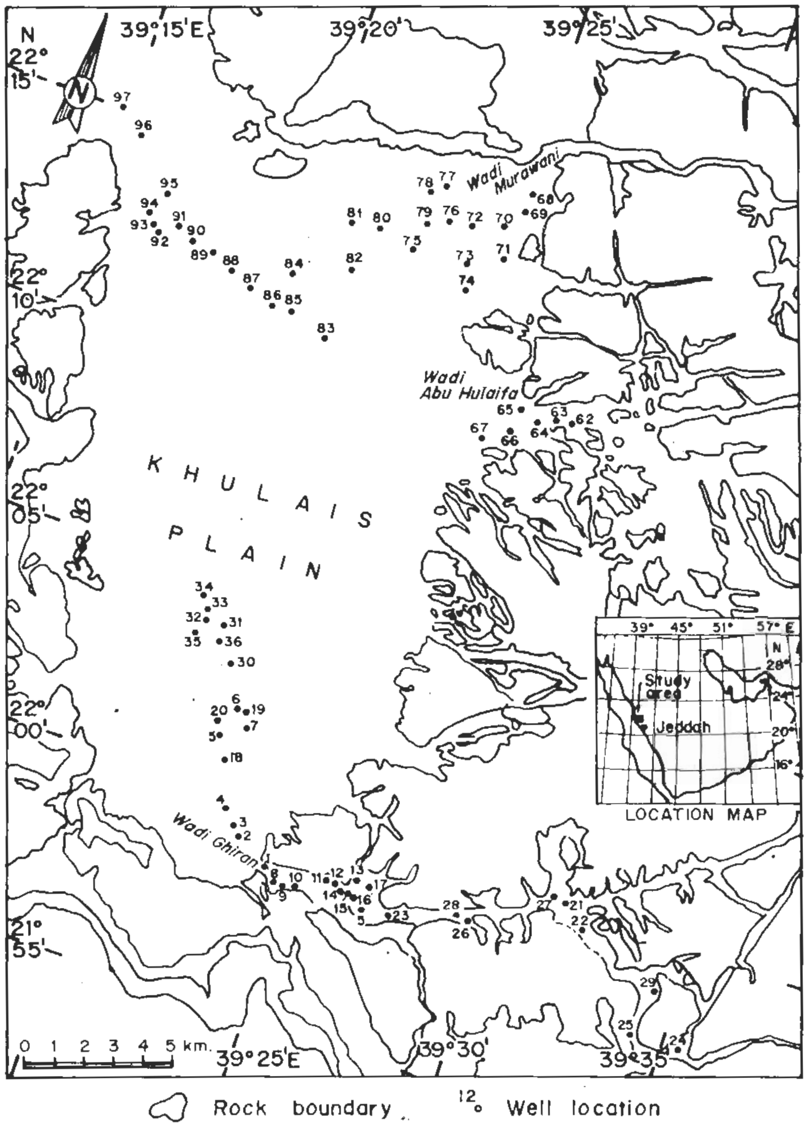

FIG. 1. Location map of study area.

in the Arabian Shield during Upper Tertiary; (3) Tertiary sedimentary cover that consists of marine and continental sediments. According to Bahafazallah *et al.* (1983), Usfan Formation is considered a dominant part of these sediments. It mainly consists of sandstone, fossiliferous limestone and shale. (4) Basement complex is represented by a group of volcanic rocks subjected to a series of deformations which resulted in tight folding and metamorphism. These rocks are of Precambrian age (Fig. 2).

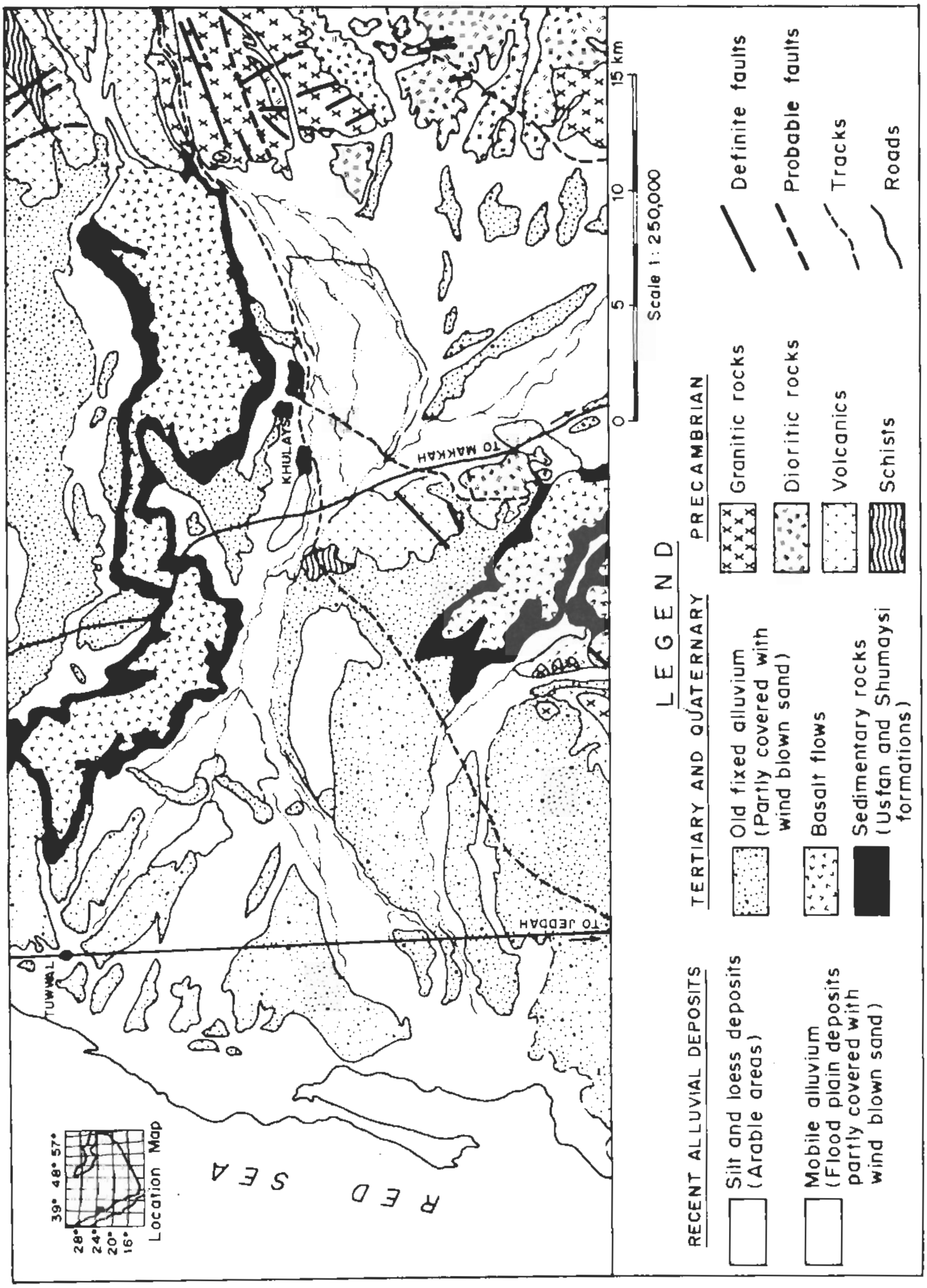

FIG. 2. Geological map, Khulais area.

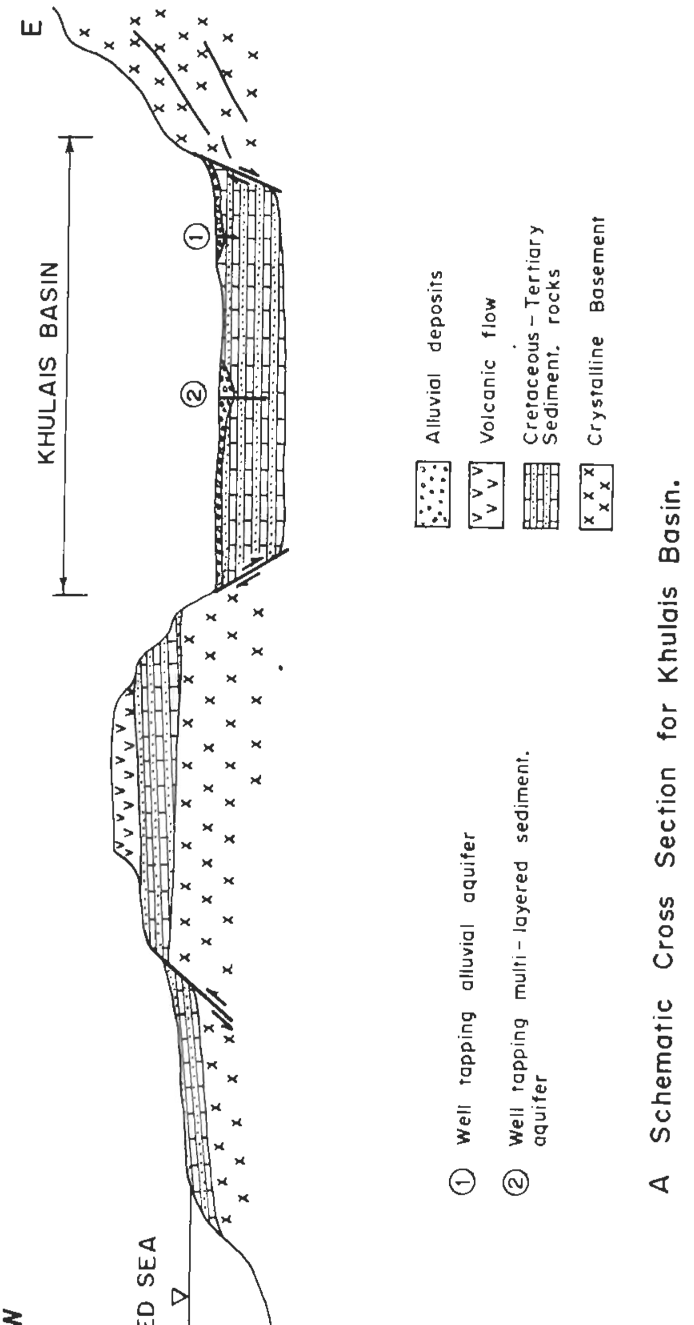

FIG. 3. Schematic geologic cross-section, Khulais area.

Groundwater occurs within two main aquifers, the alluvial deposits of the wadi system and water-bearing horizons within the clastic sedimentary succession of Cretaceous-Tertiary age (Fig. 3). The alluvium groundwater is under free surface condition while the multi-layered aquifer is under confined to semiconfined conditions.

Procedures

The 68 groundwater samples described herein were taken from wells that are situated in Khulais plain (Fig. 1). These water samples were collected over five weeks in May and June 1991. Nearly, all of the sampled wells were private domestic supply. Samples were analyzed for the major ions. Electrical conductivity (EC), pH, and temperature (°C) were measured at all the wells after it had been pumped for at least 5-10 minutes. Variables used are Ca, Mg, Na, K, SO_4, HCO_3, Cl, EC, pH and temperature. All chemical constituents are in mg/l. The saturation indices for calcite, dolomite and gypsum as well as the partial pressure of carbon dioxide (P_{co_2}) were also determined by using "WATSPEC" program written by Wigley (1977). Factor analysis was performed with the help of SPSS program (1990).

Factor Analysis (R-Mode)

Prior to factor analysis, the data were standardized to remove the effects of using different units in describing the various variables, and so the variables are put in standard form. The standardized value then has a mean value of zero and standard deviation of unity. The first stage in the FA is to compute a correlation matrix, which is a measure of interrelation for all variables. These correlation coefficients are then arranged and allows FA to compare and group the variables according to linear correlation coefficient. This type of analysis is called R-mode factor analysis, which employed in this study, with iterations of Nie *et al.* (1975). Kaiser normalization and varimax rotation were used. This is considered one of the most commonly used methods for orthogonal rotation, and results in factors that are uncorrelated. Finally, the factors' scores were calculated for each sample (Klovan 1975) and reflect the importance of given factor at that sample site. The set of scores obtained has a mean of zero and standard deviation of one. Dalton and Upchurch (1978) pointed out that factor scores can be related to each process-response described by each factor variables. They reported that negative values of factor scores reflect areas basically unaffected by the process, whereas, positive values almost represent areas affected. However, factor scores can be mapped for each factor and define the aerial distribution of the process represented by the factor.

Results and Discussion

The FA results for the groundwater samples are shown in Table 1. The FA technique gives factors in an equal number of variables employed. In practice, it is often difficult to choose the proper number of factors to retain. However, from the apparent large change in eigenvalues, it appears that three factors were retained. The *three common factors* account for 85.1% of the total variance, whereas, the other factors account for 14.9% of the total variance. Therefore, these three factors are assumed to represent, adequately, the overall variance of the data set. On the other hand, the factor loadings in Table 1 indicate that the first two factors (1 & 2) have a hydrochemically meaningful that seem to describe the existing condition of groundwater chemistry. For obtaining an interpretation of the nature of the retained factors for the system being studied, the three factors will be discussed below:

TABLE 1. Loading of elements in each factor.

Variables	Factor 1	Factor 2	Factor 3
EC	0.918	- 0.025	- 0.075
SO_4	0.917	0.011	- 0.042
Cl	0.889	- 0.213	- 0.157
Ca	0.874	0.339	- 0.097
Sat. Ind. (Gypsum)	0.871	- 0.252	- 0.062
Mg	0.863	- 0.206	- 0.033
Na	0.848	- 0.261	- 0.172
K	0.766	0.120	- 0.091
Sat. Ind. (Calcite)	- 0.147	0.947	0.082
Sat. Ind. (Dolomite)	- 0.177	0.884	0.122
P_{co_2}	0.266	- 0.833	0.121
pH	- 0.424	0.816	- 0.008
HCO_3	- 0.205	0.781	- 0.152
Temp.	0.436	0.514	0.933
Eigenvalue	6.640	4.260	1.020
Percent of Variance	47.400	30.400	7.300
Cumulative Variance	47.400	77.800	85.100

Factor 1 : accounts for 47.4% and represents the major part of the variance that reflect high loading for EC, SO_4, Cl, Ca, saturation index of gypsum, Mg, Na and K. These combinations of variables indicate that factor 1 can be associated with groundwater of high concentration of the above mentioned variables. In other words, factor 1 displays highly mineralized water effectively derived from the evaporation and dissolution processes. Comparatively low potassium loads in this factor column might be due to its release into groundwater by chemical weathering reactions of K-feldspar.

Factor 2 : accounts for 30.4% of the total variance. Saturation indices of calcite and dolomite, P_{co_2}, pH, and HCO_3 show high loading in this factor. These variables almost control the precipitation and dissolution of carbonate minerals. Temperature, Na and Ca relatively have also an effect on this factor (Table 1). The secondary loading of these three variables may indicate that ion exchange mechanism has influenced the Na and Ca concentrations, whereas temperature might control the calcite precipitation and dissolution. The high loading of bicarbonate could be attributed either to its release during the chemical weathering reactions of silicate minerals and/ or resulted from calcite dissolution by recharge water. On the other hand, the inverse relationship between pH and P_{CO_2}, which is expected in a natural water system can be readily observed in their values in this factor (Table 1).

Factor 3 : indicates that temperature is largely independently controlled and describes a unique factor assumed to be uncorrelated with each other and with the common factors. However, these variables show that it also loads moderate association

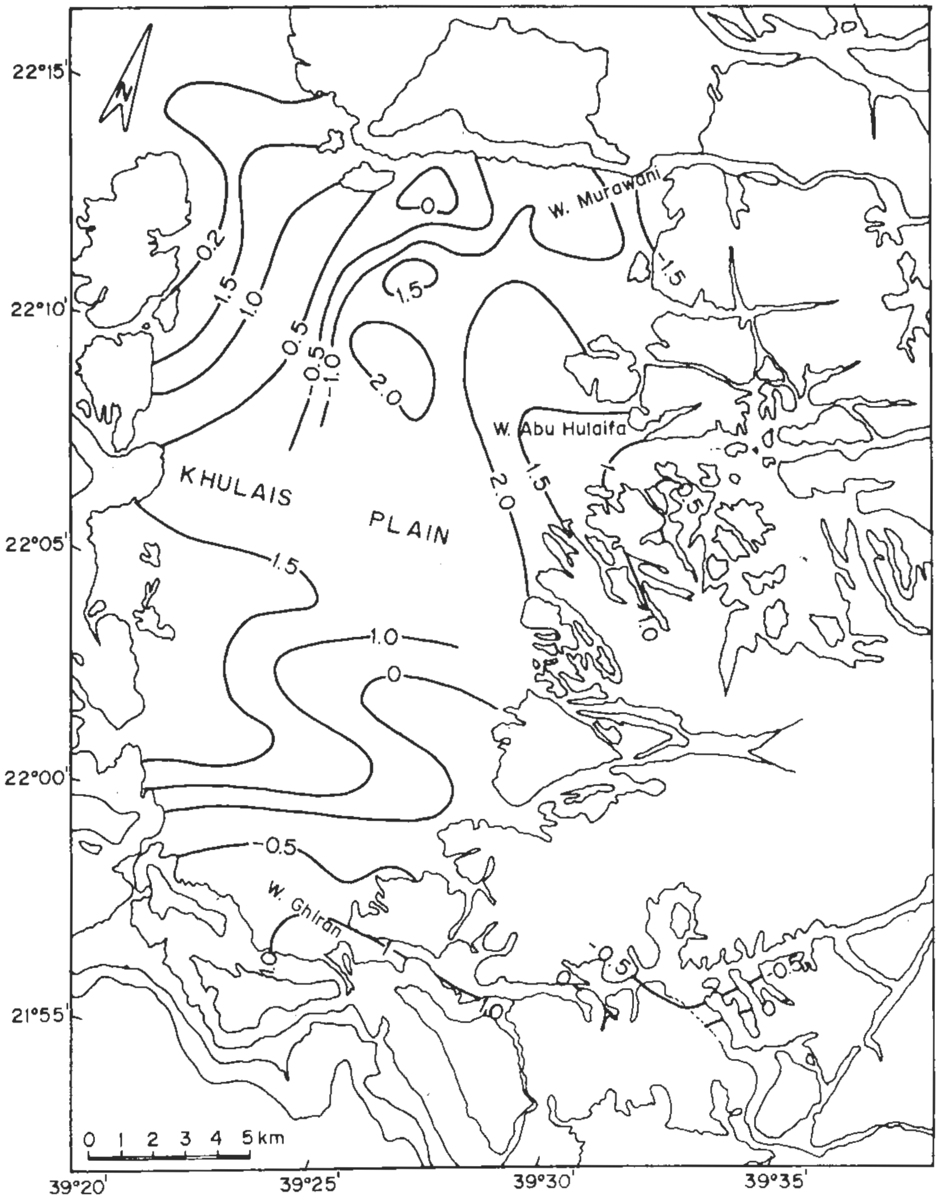

FIG. 4. Factor 1 scores distribution map.

on more than one factor (Table 1). Such condition usually interprets involvement in more than one process as mentioned above.

To delineate the area affected by the process response defined in factor 1 for each of the 68 samples, the scores were plotted and contoured in form of a spatial distribution map of factor scores (Fig. 4). It is interested to notice that the spatial variability of factor 1 confirms more or less the electrical conductivity distribution map (Fig. 5).

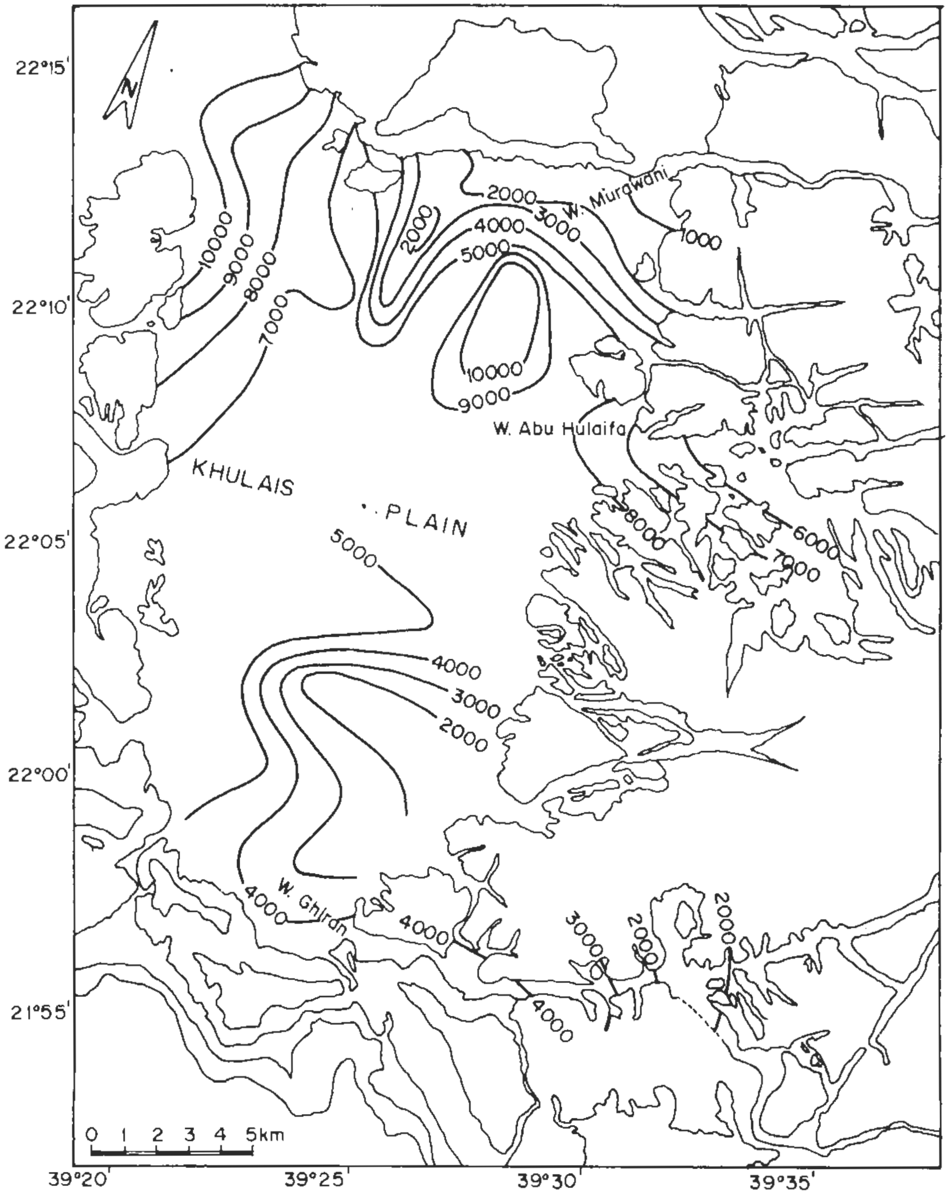

FIG. 5. Electrical conductivity distribution map.

High mineralized zones are mainly found towards the northwest corner of the study area, Wadi Abu Hulaifa, and in the downstream part of Wadi Murawani. These zones are characterized by high score (+ve sign) values of factor 1. Relatively low mineralized areas of Wadi Ghiran, the southern portion of the study area, and the upstream part of Wadi Murawani are characterized by low score (– ve sign) values of factor 1. The lack of samples, due to absence of water wells, towards the center of the plain may have obliterated the picture to some extent. The distribution of factor 1 helps, therefore, in the identification of highly mineralized zones which were outlined previously (Fig. 5) Bazuhair *et al.* (1992).

Conclusion

Factor analysis technique as used here appears systematically to reveal basic hydrochemical features. The results indicate that two types of processes reflect the groundwater chemistry condition in the Khulais basin. The first type of process is characterized by high concentration reflects highly mineralized water described by factor 1, and the second type shows the precipitation and dissolution of carbonate minerals. The hydrochemical processes outlined in this study have also been postulated as the mechanism responsible for the observed hydrochemical patterns. The application of FA demonstrates that, this technique is able to reflect the most relevant mechanism that took place in the area under study.

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تفسير كيمياء الماء الجوفي باستخدام تقنية التحليل العاملي

محمود سعيد اليماني ، عبد الغفار سعيد بازهير و محمد طاهر حسين
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المستخلص . طُبق التحليل العاملي على بيانات لكيمياء الماء الجوفي في حوض خُلَيْص بالمنطقة الغربية من المملكة العربية السعودية بغرض تقييم مدى فائدة هذه الطريقة في تفسير العمليات الكيميائية المائية . أوضحت الدراسة ظهور ثلاثة عوامل . أهم هذه العوامل التي سادت في منطقة الدراسة هي : (١) تمعدن الماء الجوفي بسبب التبخر وإذابة المعادن و (٢) عمليات إذابة وترسيب المعادن الجيرية . ويساعد التحليل العاملي أيضًا في تحديد المتغيرات المستقلة وفي تحديد نطاقات التمعدن العالي التي تمّ التعرف عليها في أعمال سابقة .