

*Short Communication*

# Profiling Water Quality Using the Multivariate Chemometric Method

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*Received: 15 April 2013*

*Accepted: 2 October 2013*

## Abstract

Water is a jewel of our Earth. Purity of water should be maintained for healthy living. Due to industrialization, the environment is polluted and the purity of water is lost. Various parameters are used for testing the quality of drinking water and for the present study electrical conductivity, pH, TDS, chloride, and total hardness of the ground water at Gerugambakkam industrial area in Chennai, India, have been measured. Our aim is to identify if the quality of tested water is acceptable or not for drinking. As multivariates are present, principal component analysis, a widely used method in chemometry is employed for ground water profiling.

**Keywords:** water quality, principal component analysis, chemometry, multivariate, ground water

## Introduction

Water is essential for all life. River and ground water are major resources and due to industrialization the effluents pollute water. In India, water is worshipped and various festivals like Kumbhmela signify the importance of maintaining the purity of it. Ground water is not only used for drinking but also for various industries such as food and pharmaceutical production, where quality of water is vital.

Indian standards has specified nearly 34 parameters for drinking water quality. Studies on water from river, ground, and coastal regions have been carried out to ascertain its quality. River water [1-4] can be tested with several chemical parameters [2] such as pH, electrical conductivity, methyl orange alkalinity, suspended solids, chloride [Cl], ammonia nitrogen, dissolved oxygen, nitrate-nitrogen, biological oxygen demand, permanganate value etc., and using physical parameters such as temperature, flow

rate, turbidity, color, etc. Both Physical and chemical parameters combined with chemometry can be applied for classification [2] and water quality identification [3]. Fuzzy logic [4, 5] along with microbial contamination [4] is used to find the water quality index of the river water. Multivariate [6] technique is employed to compare river and lake waters of the same geographical area using physico-chemical properties.

20% of the world's water resource is from ground water [7], and several measures are required to protect it. Water quality index as a measure to ensure the quality before and after the monsoon [8] periods will help to identify its purity. Ground water collected from tube wells [9] and a correlation matrix can be used to detect the correlation of physical and chemical properties of water.

Coastal water requires attention as algal growth is harmful and indirectly affects fishing and tourism. Data mining [10] techniques are employed to identify the quality of coastal water. As water quality parameters are enormous, multivariate [11] with PCA [12] can be used for parameter reduction and identification of principal parameters.

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## Experimental Procedures

### Study Area

Water samples from Gerugambakkam Industrial Area in Chennai, Tamilnadu, India were taken for analysis. This is located at 13.003N latitude and 80.13E longitude and it is an urban city on the shores of Coromandel Coast. Nearly 50 industries of different kinds are present and a few food and beverage, and pharmaceutical companies are located there.

### Sample Collection

Three bore wells from food, beverage and pharmaceutical industry location (Gerugambakkam) were taken for analysis, from each location 10 samples for 10 days (1/3/2013-12/3/2013, excluding Sundays) were collected. A total of 30 water samples from the above bore wells were collected in sterilized bottles of one litre capacity. The locations are M/s Lux Flavours Unit I, M/s Lux Flavours (Food Powder) Unit II, and M/S Kaushik Therapeutics (P) Ltd, respectively.

### Parameters Tested

(pH, Electrical Conductivity, TDS, Cl, Total Hardness)

pH measures acidity of the water based on hydrogen ion concentration and for analyzing it, a digital pH meter was used. Electrical conductivity measures the dissolved ions in water, which means the ability of the material to conduct electrical current through it. An electrical conductivity meter was used for testing. Total dissolvable solids (TDS) is the total amount of dissolved solids in water, and a TDS Meter (Deep Vision) was used for detection. Chlorides is the presence of Cl and similarly total hardness indicates the total dissolved calcium and magnesium salts in water. Titration was done for testing cl and total hardness by using Argentometry and EDTA methods, respectively.

## Results

All 30 samples were tested for the five parameters and the average of the results is given in Table 1. Indian standards (IS:10500) is widely adopted for profiling the quality of water in India. Drinking water standards from IS:10500 for the above 5 parameters is given in Table 2.

Table 1. Results of 5 parameters for water quality profiling.

Samples	pH	Elec. cond ( $\mu\text{s}/\text{cm}$ )	TDS (ppm)	Chlorides (ppm)	Total hardness (ppm)
A	5.9	460	760	456	650
B	5.8	420	725	468	630
C	5.3	438	689	488	641

Table 2. Indian standard (IS:10500)for drinking water.

pH	Elec. cond ( $\mu\text{s}/\text{cm}$ )	TDS (ppm)	Chlorides (ppm)	Total hardness (ppm)
6.5 to 8.5	300	500	250	300

Fig. 1 shows the result of the parameters indicated by bars, and the line shows the permissible limit specified by the Indian standard (IS:10500). The pH value is less compared to other values, hence the bars are not seen.

## Discussion of Results

The pH results from the Table 1 indicate that the water is acidic and it could be due to the lack of lime stones and sample C is highly acidic when compared to the other samples. As pH is less than 6.5, it tends to increase the dissolved metals such as copper, lead, iron, etc., and also leads to the corrosion of pipelines. Electrical conductivity and TDS are above the permissible limit and so the water is unhealthy for drinking. Chlorides when it is present in excess gives a salty taste. The total hardness is due to the calcium and magnesium salts in water and the excess leads to scale deposits

A database is created to store the analyzed water results. A small GUI based profiling program is written to compare the result with the Indian standard. If the values are within the acceptable range then it is displayed as acceptable; otherwise it is displayed as not acceptable.

### Algorithm for Water Analysis

Step 1: Start.

Step 2: Analyze water sample and store the result in water database.

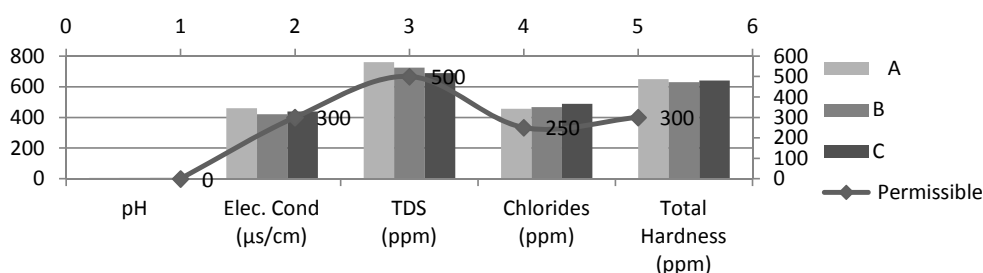


Fig. 1. Chart showing the tested parameters for water and the permissible limit given by Indian Standard IS:10500.

Table 3. Output for all the parameters from the water profiling program.

pH			Elec. conductivity			TDS			Cl			Total hardness		
A	B	C	A	B	C	A	B	C	A	B	C	A	B	C
5.9	5.8	5.3	460	420	438	760	725	689	456	468	488	650	630	641
Not Acc	Not Acc	Not Acc	Not Acc	Not Acc	Not Acc	Not Acc	Not Acc	Not Acc	Not Acc	Not Acc	Not Acc	Not Acc	Not Acc	Not Acc

Table 4. PCA analysis of water samples.

Variables	Components				
	1	2	3	4	5
pH	0.0069	-0.0084	-0.0195	-0.9944	0.1033
Elec. conductivity (µs/cm)	0.3204	0.8179	-0.4735	0.0113	0.0637
TDS (ppm)	<b>0.857</b>	-0.2717	0.1657	0.0467	0.4025
Chlorides (ppm)	<b>-0.3792</b>	0.2393	0.2726	0.078	0.8477
Total hardness (ppm)	0.1379	0.4471	0.8207	-0.0525	-0.3236
Variance	1681.4613	341.9764	0	0	0
Variance %	83.0992	16.9008	0	0	0
Cum %	83.0992	100	100	100	100

Step 3: Compare Indian standard value with the stored values from the database.

Step 4: If the range is within the acceptable limit, report as acceptable, otherwise not acceptable.

Step 5: Stop.

The output from the water profiling program is given in Table 3. It shows that all the parameters are not within the range of permissible limits and hence not acceptable (Not Acc) for drinking.

### Principal Component Analysis

Principal component analysis [12] is a decomposition technique that is employed for identifying the principal components for given data. PCA computed using xlminer and the results of analysis are given in Table 4. While analyzing the results from Table 4, if the cumulative variance is more than 80% then that component is enough for consideration. From Table 4, it is shown that from the second component the cumulative percentage is the same (100%). Hence it can be noted that only the first component can be considered for analysis. On considering the first component, higher variance is for TDS with 0.85 and Cl -0.37 (negative sign is omitted), and variance for other parameters is much less. Hence the quality of water can be well differentiated by taking the first two parameters having higher variance, i.e., TDS and Cl. The reason for increased TDS and Cl is because the region is close to the coastal area.

### Conclusion

By analyzing the five parameters for the water sample, the results indicate that the ground water from the above sites cannot be directly used for drinking, food, or pharmaceutical production. If directly consumed for drinking, it may lead to various waterborne diseases and for industry they will not get the expected quality. So it is required to purify the water before consumption. In the future we plan to test water quality from different regions in India with various parameters using chemometry.

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