



## Physicochemical assessment of groundwater quality at Kashipur (Uttarakhand) industrial areas

S Nandi\*, A Sharma, S Ahmed & D Teotia

Department of Pharmaceutical Chemistry, Global Institute of Pharmaceutical Education and Research,  
Affiliated to Uttarakhand Technical University, Kashipur – 244 713, India

\*[E-mail: sisir.iicb@gmail.com]

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The quality of groundwater has been degrading due to municipal sewage, industrial pollutants, fertilizers, herbicides, and pesticides. These dangerous pollutants enter into the deeper soil layers, infiltrate some aquifers, and decrease the gradation of groundwater. Other problems are associated with the leakage of sewer, faulty septic tank cleaning, landfill leachates, throwing of garbage into the river, pond and soil pollution. In coastal areas, salt water intrudes into fresh-water aquifers due to intensive pumping of fresh groundwater. In the present study, the city Kashipur in the state of Uttarakhand has been chosen due to big industrial settlements. The industrial wastes contain many highly harmful elements which destroy the quality of groundwater in the adjacent areas. Therefore, it is our target to test the groundwater quality of Kashipur industrial areas. To analyze the groundwater and to assess the impact of groundwater pollution of Kashipur area, an attempt has been made in the present study to test the physicochemical parameters including pH, total hardness, alkalinity, chloride, fluoride, sulphate, iron, zinc, copper and heavy metal atoms such as lead, arsenic etc. Imbalance of these parameters may degrade the quality of groundwater and may be deleterious to the health of individual and society in context of drinking, agriculture and industrial purposes. Physicochemical treatment of groundwater samples collected in summer, rainy season and post-monsoon were compared and analyzed by regression modeling making a quantitative correlation between pH and other parameters including total hardness, alkalinity, chloride, sulfate, fluoride and copper using multiple linear regression methods.

**[Keywords:** Physicochemical parameters, Treatment of groundwater quality, Quantitative pH modeling, Kashipur (Uttarakhand) industrial belt]

### Introduction

In recent years, the overpopulation and industrialization stand as the major burden on the enhanced uses of land and water resources. Groundwater is an indispensable natural resource and is situated beneath the earth. Due to underground, the general public is not so aware with groundwater than rain and surface water which are visible components of the water cycle. It is the major source of drinking water in both urban and rural areas<sup>1</sup>. Groundwater is the richest source of water supply for drinking, irrigation, and industrial purposes<sup>2</sup>. Groundwater can fulfill 23 % of all irrigation requirements, meet 53 % of all public water supplies and feed 97 % of all rural domestic water demands. The large scale industrialization has also generated a large number of toxic substances in the form of effluents<sup>3-4</sup>. These effluents pollute groundwater. Once groundwater is contaminated, it is really difficult even by expending money, time and efforts to restore it back to its original status and if we are not serious to take care it

may remain in an unstable or even hazardous condition for decade or centuries<sup>5</sup>. Hence regular monitoring of the quality of groundwater is an urgent need. There were many studies which reported the negative impact of various industries on groundwater quality<sup>2-4, 6</sup>.

Kashipur is an industrial belt with many sectors. The Government of Uttarakhand, since its inception, has paid a great attention to develop the State. An attempt has been made to take care of the water for welfare. To protect groundwater and to prevent the groundwater pollution of Kashipur area, an attempt has been made in the present study to carry out qualitative and quantitative treatment of the physicochemical parameters including total hardness, alkalinity, chloride, fluoride, sulphate, iron, zinc, copper and heavy metal atoms such as lead, arsenic etc. Imbalance of these ions may produce pathophysiological problems. Oral administration of alkaline ionized water reduce adverse side effects of hemodialysis, improves the pathological conditions

associated with bladder stone, for treating gastrointestinal tract disorders, such as gastric hyperacidity, diarrhea, etc. but water with pH higher than 10 causes skin, eye, and gastrointestinal irritation in sensitive persons. High level of chloride leads to hyperchloremia. It produces fluid retention, hypertension, muscle weakness, spasms, cardiac arrhythmia, confusion, loss of mental concentration, personality changes, numbness or tingling, seizures and convulsions. Excess fluoride in drinking water can cause dental fluorosis and skeletal fluorosis. High concentration of sulfate in the drinking water can cause catharsis that can lead to dehydration. High level of iron can lead to hemochromatosis characterized by cirrhosis of the liver, diabetes mellitus, osteoarthritis, gall bladder disease, chronic fatigue, joint pain, irregular heart beat and heart flutters. Abnormal concentration of copper leads to the Menkes' disease and Wilson's disease. Copper deficiency can cause Menkes' kinky hair disease which is characterized by poor growth and unusual "kinky" hair texture. Wilson's disease caused by chronic copper poisoning leads to the accumulation of copper predominantly in the liver and brain. Deposition of heavy metals like lead and arsenic is very dangerous because it may cause neurological damage to the babies. Elevated level of arsenic in drinking water can cause arsenicosis or arsenic poisoning. It leads to the skin problems (dermal lesions such as hyper-pigmentation and hypopigmentation), skin cancer, cancers of the bladder, kidney and lung, peripheral vascular disease (blackfoot disease), type-2 diabetes, hypertension and reproductive system abnormalities.

Imbalance of these parameters may degrade the quality of groundwater and it may produce a negative impact on the health and society in context of drinking, agriculture and industrial purposes since water is life and the degradation of ground water is a big issue in lieu of natural ecological imbalance. This kind of related work was hardly done in Kashipur industrial areas. Therefore, studies in this direction give a significant impact for the mankind.

## Experimental section

### Description of the study area

Kashipur city is situated in the Udham Singh Nagar district of Uttarakhand in India. It is famous for the pharmaceutical and paper mill industries which produce detrimental chemicals. Industrial effluents

are being thrown into the ponds and rivers. This may degrade the quality of groundwater in the vicinity. The deterioration in physicochemical and biological properties of groundwater may hamper the mankind.

### Collection of groundwater samples

Kashipur industrial belt is surrounded by Agron Remedies Pvt Ltd Moradabad Road, India Glycols Ltd Bazpur Road, The Bazpur Coop. Sugar Factory Ltd. Distillery Unit, Bazpur, M/s Sidharth Paper Ltd 7 km Moradabad Road, Shree Shayam Pulp & Board Mills Ltd. Unit II, Moradabad Road, M/s Siddheshwari Paper Udyog Ltd 7 km Moradabad road, Prolific papers (P) Ltd. 5 km stone, Aliganj Road, Kashipur, Devrishi paper Pvt Ltd., Jaspur Road, Jagatpur Patti, Jaspur, Vivimed Lab Pvt Ltd Kashipur.

Water samples from hand pumps and submersible wells were collected from different surrounding industrial places in summer (in the mid of May 2018), monsoon (mid of August 2018) and post-monsoon (3<sup>rd</sup> week of September 2018). The samples were procured in pre-cleaned laboratory borosilicate reagent bottles and capped with the stopper. The room temperature (25 °C to 35 °C) was maintained with necessary precautions. The samples were being tested to compute the physicochemical parameters within two days from the date of collection of the water utilizing standard methodologies.

Standard methods<sup>7-8</sup> were applied for the assessment of total hardness, total alkalinity, chloride, sulfates, iron, heavy metal atoms such as lead, arsenic etc., fluoride, and copper. Normal limit of these elements is given as 175-358 ppm, 231.8-542.8 ppm, 50-350 ppm, 200-250 ppm, 0.18-1.59 ppm, 0.02-0.08 ppm, 0.010 ppm, 0.7-1.9 ppm, and 0.017-0.061 ppm respectively<sup>8</sup>.

### Methods of testing the water samples

#### Calculation of total hardness (TH)

The hardness of water is a measure of the total concentration of the bicarbonate, chloride, and sulfates of calcium and magnesium. Water hardness is caused by excessive multivalent metal ions which come from minerals dissolved in the water. Hardness is judged based on the ability of these ions to form a precipitate or soap scum upon reacting with soap. So far as reported, hard water is not harmful to the health and soft water causes cardiac problem<sup>2,4,9</sup>. Total hardness of the water samples was calculated using volumetric

titration method which considers Eriochrome Black T (EBT) as an indicator and EDTA as titrant. The test is carried out in accordance with IS: 3025 (Part 21) – Reaffirmed 2002<sup>(ref. 10)</sup>.

#### *Calculation of total alkalinity (TA)*

Total alkalinity in water is caused by hydroxyl, carbonate and bicarbonate ions. A large amount of alkalinity produces bitterness in taste. The water alkalinity can be determined by titrating the water sample with sulphuric acid of known pH, volume and concentration. Based on the stoichiometry of the reaction and number of moles of sulphuric acid needed to reach the endpoint, the concentration of alkalinity in water is calculated. Phenolphthalein, methyl red, and bromocresol green are used as a mixed indicator in the present experiment. The test is given in IS: 3025 (Part 23) – Reaffirmed 2003<sup>(ref. 11)</sup>.

#### *Qualitative estimation of chloride, sulfates, iron, heavy metal atoms such as lead and arsenic*

The limit test was carried out for the qualitative detection of impurities and to control small amount of impurity present in the water samples. Even, the presence of a very minute quantity of the impurity may produce cumulative toxicity and harm the health. So, the limit test is applied to identify the impurities present in the pharmaceutical substance and compare it with standard and check whether the sample contains the number of impurities above the limit or within the limit. In the present study, limit tests for the qualitative estimation of chloride, sulphates, iron, heavy metal atoms such as lead and arsenic were being carried out by the standard methodologies as prescribed in Indian Pharmacopoeia 2016<sup>(ref. 8)</sup>.

Limit test for chloride considers the reaction between soluble chlorides and silver nitrate in the presence of dilute nitric acid to produce white opalescence of silver chloride. Limit test for sulphate considers the reaction of soluble sulphate with barium chloride in the presence of dilute hydrochloric acid to produce barium sulphate with turbid solution. Limit test for iron is based on the reaction of iron in ammonical solution with thioglycolic acid in the presence of citric acid to produce pale pink to deep reddish purple colored solution of iron thioglycolate. Heavy metals such as lead and arsenic produce cumulative toxicity which hampers the nervous system in children. Presence of heavy metals above the limit in food and drinking water is very dangerous for the health. The limit test for lead is based on the

reaction between the solution of lead and a saturated solution of hydrogen sulphide. In acidic media, it produces reddish/ black color with hydrogen sulphide which is compared with standard lead nitrate solution. Limit test for arsenic can be carried out using Gutzeit apparatus which considers the reaction between arsenic gas and hydrogen ion to form yellow colored stain on mercuric chloride paper in the presence of potassium iodide as reducing agents. Arsenic is present as arsenic acid in the sample. It is reduced to arsenious acid by reducing agents like potassium iodide, stannous acid, zinc, hydrochloric acid, etc. Arsenious acid is further reduced to arsine gas by the nascent hydrogen and then reacts with mercuric chloride paper to give a yellow stain<sup>8</sup>.

#### *Test for fluoride*

Fluoride is omnipresent in minerals and in geochemical deposits. It is generally leached into subsoil water sources by slow natural degradation of fluorine contained in rocks. If fluoride is present above the normal limit, the water causes serious health hazards such as dental, skeletal and non-skeletal fluorosis. Potable water is tested to control fluoride level in the water. In the present study, Aqua check fluoride testing kit WT012 has been used for the determination of fluoride content present in the water samples. Aqua check fluoride testing kit WT012 contains two reagents such as 012A and 012B respectively. 10 ml of the water sample was taken in a test tube jar. 3 drops of reagent 012A and 8 drops of reagent 012B were being added simultaneously and mixed well using a glass rod and then it is being allowed for 4-5 minutes. Level of the fluoride content was noted from the provided chart by making a comparison with the standard color (Fig. 1A) and the color developed in the test tube<sup>12</sup>.

#### *Test for copper*

Copper occurs naturally in rock, soil, water, sediment, and air. It is commonly found in coins, electrical wiring, and pipes. It is an essential element that should be taken through the diet to ensure good health. However, too much copper can cause adverse health effects, including vomiting, diarrhea, stomach cramps, and nausea. It has also been associated with liver damage and kidney disease<sup>13</sup>. In the present study, copper testing kit WT046 containing 046A and 046 B reagents are used to check the level of copper in groundwater samples. In the method, 10 ml of the water sample was taken in a test tube jar. 2 drops of reagent 046A and 1 drop of reagent 046B were being

added simultaneously and mixed well using a glass rod and then allowed the test tube to rest for 5-10 minutes. Level of the copper content was checked from the provided chart by making a comparison with the standard color (Fig. 1B) and the color developed in the test tube<sup>12</sup>.

**Measurement of the pH**

pH meter can measure pH of the samples. It determines the hydrogen-ion activity in aqueous solutions, indicating its acidity or alkalinity expressed as pH. The pH meter measures the difference in electrical potential between a pH electrode and a reference electrode. The difference in electrical potential relates to the acidity or pH of the solution<sup>14</sup>.

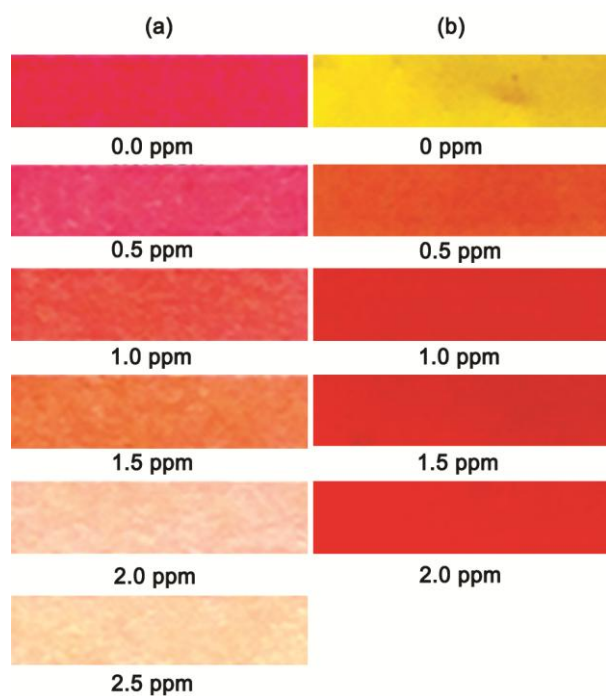


Fig. 1 — A-B: Standard fluoride color chart (1A) and standard copper color chart (1B)

**Results and Discussion**

In the mid of May 2018, 1<sup>st</sup> phase groundwater samples were collected from submersible pumps of the different locality enlisted in the Table 1.

These samples were subjected to the testing of pH, total hardness, alkalinity, limit test for chloride, sulfate, iron, lead and arsenic and test for fluoride and copper. Samples were tested as per the standard methods. The contribution of different physicochemical parameters is represented by indicator variables, which occupy the value of 1 or 0 if the corresponding parameter is within or above the limit. The results were summarized in Table 2. Table 3 denotes the parameter value as obtained from the corresponding tests. Iron, lead, and arsenic contents are within the limit and indicated in the bold in Table 2 for all the samples.

Physiochemical data of water samples of summer season reveals that iron, lead, and arsenic content in all the water samples are within the limit as highlighted in the above Table 1 while sulphate, chloride, fluoride and copper level are above the limit in some localities. Sulphate level of most of the water samples except S6, S8, and S9 are above the limit. Amount of the chloride ions present in the samples S3 and S7 are not within the permissible limit. Total hardness for sample S4 is below the limit whereas

Table 1 — List of samples collected from submersible pumps of the different locality (summer season)

Sl. No.	Sample	Locality
1	S1	Sugar Mill, Kashipur
2	S2	Pashupati Polytex
3	S3	Agron Remedies Pvt. Ltd and Anaj Mandi
4	S4	Kunda Chowraha
5	S5	India Glycol Limited
6	S6	Maldhan residential area
7	S7	Government hospital Kashipur
8	S8	Vivimed Lab Ltd Kundeshwari
9	S9	Surya Roshni Limited, Moradabad road

Table 2 — Calculated physicochemical parameter data of groundwater of different Kashipur industrial zone (summer)

Sl. No	Total Hardness	Total alkalinity	Chloride	Sulphate	Iron	Limit test			Fluoride	Copper	pH
						Lead	Arsenic				
S1	1	1	1	0	<b>1</b>	<b>1</b>	<b>1</b>	1	0	7.65	
S2	1	1	1	0	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.62	
S3	1	0	0	0	<b>1</b>	<b>1</b>	<b>1</b>	0	1	7.58	
S4	0	1	1	0	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.80	
S5	1	0	1	0	<b>1</b>	<b>1</b>	<b>1</b>	1	0	7.76	
S6	1	1	1	1	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.40	
S7	1	1	0	0	<b>1</b>	<b>1</b>	<b>1</b>	1	0	7.30	
S8	1	1	1	1	<b>1</b>	<b>1</b>	<b>1</b>	0	1	7.50	
S9	1	1	1	1	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.61	

1= acceptable (within the limit); 0 = not acceptable (above the limit)

total alkalinity content for samples S3 and S5 are below the limit. Fluoride test shows that the presence of fluoride ions in S1-S2, S4-S7, and S9 are within the limit and sample S3 and S8 contain fluoride amount below the limit. The samples S1, S5, and S7 contain copper ion an amount of 0.5 ppm, 0.5 ppm and 1.5 ppm which are not within the permeable limit. Alkalinity and hardness level was quite normal in most water samples. pH of all the water samples is slightly basic.

2<sup>nd</sup> phase water samples were collected in the mid of August 2018 from different Kashipur localities enlisted in Table 4.

Samples were tested and physicochemical parameters with or without acceptable limits were denoted by 1 and 0 digits which were tabulated in Table 5. Chloride, Iron, lead, and arsenic contents are indicated as bold in Table 5 for all the samples

Table 3 — Physicochemical parameter values (ppm) of total hardness, alkalinity, fluoride and copper (summer)

Sl. No	Total hardness	Total alkalinity	Fluoride	Copper
S1	210	258	0.50	0.50
S2	240	320	0.50	0.00
S3	200	221	0.00	0.00
S4	150	333	1.00	0.00
S5	195	216	0.50	0.50
S6	205	249	0.50	0.00
S7	305	307	0.50	1.50
S8	225	250	0.00	0.00
S9	225	255	0.50	0.00

collected in rainy season. Physicochemical parameter values of total hardness, alkalinity, fluoride and copper (Rainy season) were calculated and given in Table 6.

It was shown that total hardness data of S10, S17, S19, and S21-S23 are 370 ppm, 495 ppm, 425 ppm, 425 ppm, 480 ppm and 500 ppm. These are not acceptable because of above the normal limit. Total alkalinity of all water samples decreases from the normal level. Chloride, iron, lead, and arsenic levels were shown within the permeable limit for all the water samples. Fluoride and copper content

Table 4 — List of samples collected from different Kashipur localities (rainy season)

Sl. No.	Sample	Locality
1	S10	Sugar Mill, Kashipur
2	S11	Pashupati Polytex
3	S12	Agron Remedies Pvt Ltd and Anaj Mandi
4	S13	Kunda Chowraha
5	S14	India Glycol Limited
6	S15	Shakti Chowraha, Mahuakheraganj
7	S16	Government Hospital, Kashipur
8	S17	Vivi med Lab Kundeswari
9	S18	Surya Roshni Limited, Moradabad road
10	S19	Genesis Mahuakheraganj
11	S20	Devrishi paper mill
12	S21	Sugar Mill Nadahi
13	S22	Government hospital Jaspur
14	S23	IIM Kashipur
15	S24	Techno Electric, Moradabad road
16	S25	GIPER, Jaspur road

Table 5 — Calculated physicochemical parameter data (rainy season) of groundwater of different Kashipur industrial zone

Sl. No	Total hardness	Total alkalinity	Limit test							pH	
			Chloride	Sulfate	Iron	Lead	Arsenic	Fluoride	Copper		
S10	0	0	<b>1</b>	1	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	0	7.14
S11	1	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.23
S12	1	0	<b>1</b>	1	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	6.94
S13	1	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.65
S14	1	1	<b>1</b>	1	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.45
S15	1	0	<b>1</b>	1	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.25
S16	1	1	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.13
S17	0	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	6.89
S18	1	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.25
S19	0	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	6.71
S20	1	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.28
S21	0	1	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	6.95
S22	0	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	0	7.05
S23	0	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	0	1	7.16
S24	1	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.33
S25	1	0	<b>1</b>	1	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	1	7.10

1= acceptable (within the limit); 0 = not acceptable (above the limit)

of most water samples are within the limit while sulfate level is above the limit in most samples. pH of some samples becomes acidic during the rainy season.

3<sup>rd</sup> phase water samples were collected in the post-monsoon of the 3<sup>rd</sup> week of September 2018 from different Kashipur localities enlisted in the Table 7.

Samples were tested and physicochemical parameters with or without acceptable limit were denoted by 1 and 0 digits (Table 8). In the post-monsoon season, chloride, iron, lead, arsenic and fluoride contents are indicated as bold in Table 8 for

all the samples. Physicochemical parameter values of total hardness, alkalinity, fluoride and copper (post-monsoon) were calculated and given in Table 9.

3<sup>rd</sup> phase test results show that total hardness of the water samples such as S35, S37, and S38 has exceeded the limit. Total alkalinity is maintained below the limit for the almost 50 % of the sample tested. The level of chloride, iron lead, arsenic, fluoride, and copper are almost acceptable for all the samples. Water samples of S26, S28, S30, and S31 are not within the limit of sulphate content as per the standard limit test.

Table 6 — Physicochemical parameter values (ppm) of total hardness, alkalinity, fluoride and copper (rainy season)

Sl. No	Total hardness	Total alkalinity	Fluoride	Copper
S10	370	170	0.50	0.5
S11	290	139	0.50	0.00
S12	315	200	1.00	0.00
S13	195	131	1.00	0.00
S14	240	350	1.00	0.00
S15	325	225	0.50	0.00
S16	280	216	0.50	0.00
S17	495	214	0.50	0.00
S18	240	194	0.50	0.00
S19	425	221	0.50	0.00
S20	270	210	0.50	0.00
S21	450	248	0.50	0.00
S22	480	175	0.50	0.5
S23	500	221	0.00	0.00
S24	265	175	1.00	0.00
S25	310	172	0.50	0.00

Table 7 — list of samples collected from different Kashipur localities (post monsoon season)

Sl. No.	Sample	Locality
1	S26	M/s Sidharth Paper Ltd 7 km Moradabad road
2	S27	Prolific papers (P) Ltd. 5 km stone, Aliganj Road
3	S28	Vishvakarma Paper and Board Limited, 4.5 km, Ramnagar Road
4	S29	Nainy paper Ltd, 7 km, Moradabad road
5	S30	Sugar Mills Kashipur
6	S31	Shree Shayam Pulp and Board Mills Ltd. Unit II, Moradabad road, Kashipur
7	S32	Flexituff International Limited, Mahuakheraganj
8	S33	Konark Industries, Mahuakheraganj
9	S34	Videocon Moradabad road
10	S35	India Glycol Limited
11	S36	Agron Remedies Pvt Ltd
12	S37	Government hospital Kashipur
13	S38	Vivi med Lab Kundeswari
14	S39	Surya Roshni Limited, Moradabad road
15	S40	Genesis Mahuakheraganj

Table 8 — Calculated physicochemical parameter data (post-monsoon) of groundwater of different Kashipur industrial zone

Sl. No	Total hardness	Total alkalinity	Limit test							pH
			Chloride	Sulfate	Iron	Lead	Arsenic	Fluoride	Copper	
S26	1	1	<b>1</b>	1	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.34
S27	1	1	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.20
S28	1	1	<b>1</b>	1	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.4
S29	1	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.33
S30	1	1	<b>1</b>	1	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.35
S31	1	0	<b>1</b>	1	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.39
S32	1	1	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.13
S33	1	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	0	6.89
S34	1	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.25
S35	0	1	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	6.80
S36	1	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.20
S37	0	1	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.02
S38	0	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.15
S39	1	1	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.26
S40	1	0	<b>1</b>	0	<b>1</b>	<b>1</b>	<b>1</b>	<b>1</b>	1	7.32

1= acceptable (within the limit); 0 = not acceptable (above the limit) fluoride and copper (post-monsoon)

Table 9 — Physicochemical parameter values (ppm) of total hardness, alkalinity, fluoride and copper (post-monsoon)

Sl. No	Total hardness	Total alkalinity	Fluoride	Copper
S26	355	235	0.50	0.00
S27	295	240	0.50	0.00
S28	325	232	1.00	0.00
S29	200	140	1.00	0.00
S30	245	345	1.00	0.00
S31	320	230	0.50	0.00
S32	285	238	0.50	0.00
S33	355	225	0.50	0.50
S34	245	195	0.50	0.00
S35	430	238	0.50	0.00
S36	275	220	0.50	0.00
S37	455	245	0.50	0.00
S38	485	195	0.50	0.00
S39	350	235	0.50	0.00
S40	275	200	1.00	0.00

#### Statistical analyses

pH is an important parameter measuring acidity and basicity of any solution. It can be quantified as the negative logarithm of hydrogen ion concentration which is derived by the Henderson–Hasselbalch equation. As per the equation, pH is defined as a measure of acidity (using  $pK_a$ , the negative log of the acid dissociation constant) calculated in biological and chemical systems. The equation is also useful for estimating the pH of a buffer solution and finding the equilibrium pH in acid-base reactions. The equation is given by

$$pH = pK_a + \log_{10} \left( \frac{[A^-]}{[HA]} \right)$$

Here, [HA] is the molar concentration of the undissociated weak acid,  $[A^-]$  is the molar concentration of this acid's conjugate base and  $pK_a$  is the negative logarithm of the acid dissociation constant ( $K_a$ ). From the above equation, it is clear that pH quantitatively depends on the molar concentration of conjugate base or acid which means that it depends on the molar concentration of the Lewis acid or base in cases of corresponding standard acid or base ionization in water. Therefore, it was postulated that the pH of the groundwater depends on different anions ( $Cl^-$ ,  $SO_4^{2-}$ ,  $F^{2-}$ ) and cations such as copper, calcium, and magnesium, etc.

#### Validation of results by mathematical modeling

Therefore, in the present attempt, multiple linear regressions (MLR) analysis was performed by making a quantitative correlation between pH and other parameters including total hardness, alkalinity,

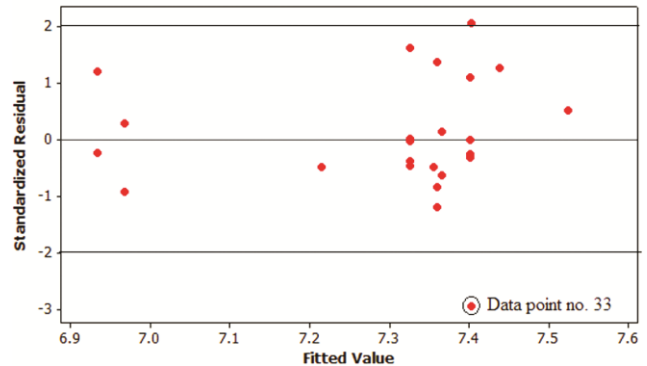


Fig. 2 — Residual vs fitted values of the response data

chloride, sulfate, fluoride, and copper using multiple linear regression methods. Minitab 17 software<sup>15</sup> was used to develop the regression model considering physicochemical data points of S1 to S40 water samples. Many models were generated with a random selection of the different percentage of training and test set<sup>16-17</sup>. The best regression equation is given by training data of 65 % and 35 % test data points (S4, S8, S10, S12, S14, S16, S19-S22, S25, S28, S36, S39) of total observations.

$$pH = 7.210 + 0.392 \text{ T.H.} + 0.0349 \text{ T.A.} + 0.083 \text{ Chloride} + 0.041 \text{ Sulphate} - 0.282 \text{ Fluoride} - 0.077 \text{ Copper}$$

$$N = 26, R^2 = 0.432, \text{ PRESS} = 1.757, S = 0.212 \dots (1)$$

Where,  $N$  is the number of observations,  $R$  is the square root of multiple  $R^2$  for regression, PRESS is the predictive sum of squared deviation, and  $S$  is the standard error of estimation.

The above model can explain only 43.2 % variances of the total data points. The result was not so good. Hence, further statistical validation was done by calculating the residual versus fitted plot of the response data (Fig. 2). The graph has shown that data point 33 does not fit within the applicability zone, so, data point 33 was predicted as an outlier.

Therefore, data point 33 has been omitted from the data points and again model was formulated which is as follows

$$pH = 7.37 + 0.403 \text{ T.H.} - 0.0209 \text{ T.A.} + 0.218 \text{ Chloride} + 0.0549 \text{ Sulphate} - 0.332 \text{ Fluoride} - 0.308 \text{ Copper}$$

$$N=25, R^2 = 0.650, \text{ PRESS} = 1.305, S = 0.161 \dots (2)$$

This model gives an  $R^2$  value of 0.650. Further, this model was used to predict the pH of the test set. Predicted pH values are given in Table 10.

Table 10 — Observed and predicted pH of the test data points

Test set	Observed pH	Predicted pH
S8	7.5	7.717
S10	7.14	7.3109
S14	7.45	7.385
S16	7.13	7.3301
S19	6.71	6.948
S20	7.28	7.351
S21	6.95	6.9271
S22	7.05	7.256
S25	7.1	7.4059
S28	7.4	7.385
S36	7.2	7.351
S39	7.26	7.3301
S4	7.8	7.6621
S12	6.94	7.4059

A correlation graph was plotted taking the data points of observed and predicted pH for the test set. It has been represented in Figure S1. The results show good predictability which was obtained by the training model Eq. 2 in terms of squared correlation coefficient ( $r^2$ ) between observed and predicted pH of the test data points shown as 0.654.

Further statistical validation has been done by calculating the T-value associated with the regression equation. It is defined as the modeled parameter coefficient divided by its standard error<sup>17-18</sup>. Physicochemical parameters with large |T| values produce significant contribution in the regression modeling of pH (Table S1).

It was found that TH, copper,  $F^{2-}$ ,  $Cl^-$ , and  $SO_4^{2-}$  produce higher |T| values of 4.36, 2.650, 2.150, 1.39 and 0.630, respectively.

## Conclusion

Three phases (summer, rainy and post-monsoon) of groundwater samples of different localities of Kashipur industrial areas were collected and subjected to testing of physicochemical parameters governing the quality of the groundwater. Physicochemical data of summer, rainy season and post-monsoon were compared. It was found that the alkalinity of water samples decreases during the rainy season and post-monsoon period, therefore, the pH of some samples became slightly acidic. Iron, fluoride, chloride, and copper level becomes normal in most water samples during the rainy season and post-monsoon. Rainy seasons' and post-monsoon' data shows that total hardness data become higher than the summer season. This is not harmful to health. The most important observation in this study is that heavy metals

like lead and arsenic were within the limit in Kashipur industrial areas. It was also observed that the quality of groundwater during rainy and post-monsoon seasons are comparatively better than the summer because rainwater penetrates through many layers of the underground soil which may act as natural filters to retain the impurities and groundwater aquifers move up to saturate the uppermost stratum. The present work gives significant impact towards ease of qualitative and quantitative estimation of different impurities to be considered as physicochemical parameters mediated groundwater quality. To further validate the data, a quantitative correlation between pH and other parameters including total hardness, alkalinity, chloride, sulfate, fluoride and copper using multiple linear regression methods was formulated where higher |T| values of TH, copper,  $F^{2-}$ ,  $Cl^-$ , and  $SO_4^{2-}$  show significant impact while considering the quality of drinking water.

## Supplementary Data

Supplementary data associated with this article is available in the electronic form at [http://nopr.niscair.res.in/jinfo/ijms/IJMS\\_49\(08\)1486-1494\\_SupplData.pdf](http://nopr.niscair.res.in/jinfo/ijms/IJMS_49(08)1486-1494_SupplData.pdf)

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## Declaration of Interest

The authors report no conflicts of interest.

## Author Contributions

AS and SA performed this work under supervision of SN. DT supported the data analyses.

## References

- 1 Pranam T S D, Rao T V, Punithavathi L, Karunanithi S & Bhaskaran A, Ground water pollution in the Palar Riverbed near Vellore Tamil Nadu, India, *Indian J Sci Technol*, 4 (2011) 19-21.
- 2 Gupta D P, Sunita & Saharan J P, Physicochemical analysis of ground water of selected areas of Kaithal city (Haryana), *Researcher*, 1 (2009) 1-5.
- 3 Jameel A A, Evaluation of drinking water quality in Tiruchirapalli, Tamil Nadu, *Indian J Env Health*, 44 (2002) 108-112.
- 4 Kethikeyani T P, Velavan T P & Ramesh M, Physico-chemical and biological characteristics of river Shanmuganadhi, *Env Eco*, 20 (2002) 482-486.
- 5 Bisnoi M & Arora S, Potable ground water quality in some villages of Haryana India, *J Environ Biol*, 28 (2007) 291-294.



- 6 Singh K P, Temporal changes in the chemical quality of groundwater in Ludhiana area, Punjab, India, *Curr Sci*, 66 (1994) 375-378.
- 7 APHA, Standard methods for the examination of water and Wastewater, (American Public Health Association/American Water Works Association/Water Environment Federation, Washington, D.C.), 21, 2005.
- 8 Indian Pharmacopoeia 2014, Addendum 2016, Indian Pharmacopoeia Commission, 7<sup>th</sup> edn, Vol 1, 2016.
- 9 Nandi S, Sharma A, Ahmed S & Teotia D, Quantitative Regression Analysis of Total Hardness Related Physicochemical Parameters of Groundwater, *Pharm Res*, 2 (2018) 000160.
- 10 <https://docplayer.net/19221801-5-0-experiment-on-determination-of-total-hardness.html>
- 11 <https://docplayer.net/39688585-7-0-experiment-on-determination-of-alkalinity-of-water.html>
- 12 [www.himedialabs.com](http://www.himedialabs.com)
- 13 <http://www.health.state.mn.us/divs/eh/water>
- 14 Pye W G, Potentiometric pH Meter, *J Sci Instrum*, 39 (1962) 323 pp.
- 15 <http://www.minitab.com>
- 16 Nandi S & Bagchi M C, QSAR of aminopyrido[2,3-d]pyrimidin-7-yl derivatives: anticancer drug design by computed descriptors, *J Enzyme Inhib Med Chem*, 24 (2009) 937-948.
- 17 Salman M & Nandi S, QSAR and pharmacophore modeling of aminopyridazine derivatives of  $\gamma$ -amino butyric acid as selective GABA-A receptor antagonists against induced coma, *Res Rep Med Chem*, 5 (2015) 49-60.
- 18 Bagchi M C, Mills D & Basak S C, Quantitative structure-activity relationship (QSAR) studies of quinolone antibacterials against *M. fortuitum* and *M. smegmatis* using theoretical molecular descriptors, *J Mol Model*, 13 (2007) 111-120.