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A mathematical approach to evaluate the extent of groundwater contamination using polynomial approximation

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ABSTRACT

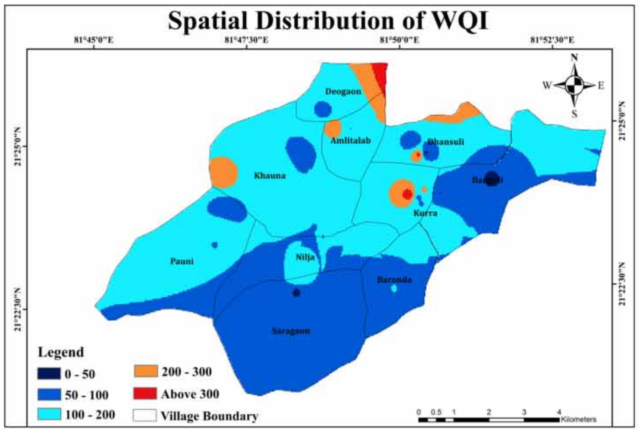
Groundwater is getting contamination rapidly due to various anthropogenic activities and geogenic sources. In this direction, assessment of water quality analysis is the basic requirement for nurturing human being and its evolution. Water Quality Index (WQI) parameter have been widely used in determining water quality globally. The study aims to provide the suitability of groundwater in the specified region using polynomial approximation method for drinking and irrigation purposes along with the computation of WQI using conventional method. Weierstrass's polynomial approximation theorem along with longitudinal and latitudinal values has been used to evaluate the polynomial regarding various physico-chemical parameters. To validate the obtained results from the present approach, groundwater water quality data collected and analyzed from the Pindrawan tank area in Raipur district, Chhattisgarh, India have been used. The result obtained i.e., the Intermediate value of the parameters obtained correctly from the mathematical modeling with an average error of 7%. This polynomial approximation method can also be used as the substitute of inverse modeling to determine the location of the source in two-dimension system. The approach output can be beneficial to administrators in making decisions on groundwater quality and gaining insight into the tradeoff between system benefit and environmental requirement.

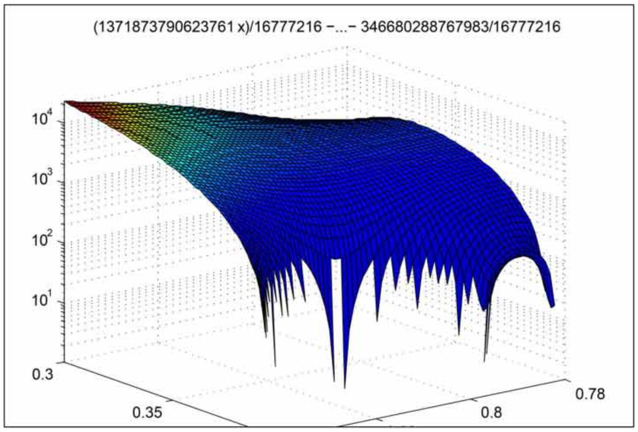
Key words: contaminant concentration, groundwater, parameter estimation, pindrawan tank area, polynomial approximation, water quality index

HIGHLIGHTS

- Approximation of contaminant concentration of groundwater for various physio-chemical parameters.
- Use of polynomial approximation in any geological scenario to predict contaminant concentration.
- Collect data for a specific region and using the data to find the values of the constants.
- Cross verify the result with observed value and 7% expected error was obtained.

GRAPHICAL ABSTRACT





1. INTRODUCTION

Groundwater is a primary source of drinking water in our country but day by day increment of groundwater contamination due to various anthropogenic activities as well as geogenic sources makes the life difficult especially for the rural people. The main question is that the available water in the bore wells/dug wells is drinkable or not? Mathematical modeling has been presented by researchers and scientists to predict the contamination level in the aquifer aquitard system. Yates (1992) used LTT to solve one-dimensional generalized Advection Dispersion Equation (ADE) in a semi-infinite domain. Logan (1996) extended the work of Yates (1992) using scale-dependent dispersion and periodic boundary conditions. Aral & Liao (1996) and Batu (1996) solved two-dimensional and three-dimensional generalized ADE respectively. Fractional ADE have been incorporated to study the impact of groundwater contamination (Benson *et al.* 2000; Schumer 2001; Marinca *et al.* 2009; Pandey *et al.* 2012; Singh & Chatterjee 2017). In the above-mentioned papers the contaminant concentration has been taken care of but the specific contaminant concentration for one element and the overall quality of the groundwater is not predicted. Often it will become difficult to predict the contaminant concentration for certain zone using ADE.

According to World Health Origination (WHO), the use of contaminated water causes around 80% of total diseases in human. Pollution in the groundwater system is a severe threat to public health as well as the economic and social life (Milovanovic 2007). Therefore, monitoring the groundwater quality and controlling the pollution level in groundwater is the need of the hour (Simeonov *et al.* 2003). Groundwater may have direct impact on agriculture as most irrigation system depends on the bore well in India. So, it is quite essential to maintain the quality of the irrigation water. Additionally, experts from all disciplines have approved that factor such as urbanization, industrialization, poor land organization, and environmental pollution-imposed bonus stress on irrigation production. These factors have a significant effect in terms of both quantity and quality of water for irrigation.

Water Quality Index (WQI) is regarded as one of the most efficient ways for the rating and classification of water quality for drinking and irrigation purposes (Brown *et al.* 1972; Ott 1978; Miller *et al.* 1986; Bordalo *et al.* 2001; Cude 2001; Hallock 2002; Agarwal *et al.* 2021a, 2021b). So, it is quite essential that author can be able to predict the WQI index for any point present at the domain of study.

Here in this present study our main goal is to approximate the contaminant concentration profile using polynomial approximation method for the whole domain using some limited numbers of data. It is often become difficult as well as costly to collect large numbers of data which are mostly used for statistical or machine learning based solutions. Depending upon the degree of the polynomial we are going to choose the number of data required, as an example one can say that we need three values to identify the two-dimensional linear curve. So, in this present paper we are not only using the polynomial approximation method to find the contaminant concentration level but also validating our work with the field data. In literature, the polynomial approximation method has not been used for estimation of pollutants in groundwater contamination problem. This is a novel approval as it is not utilized earlier in water quality studies and is first of its kind to the best of the authors knowledge. Hence, in this present study authors utilized the polynomial approximation method to predict the contaminant concentration values in different locations. Polynomial approximation method requires less number of dataset to fit the curve, but depending upon the required accuracy the number of data may be increased although less number of data also provides a good result as discussed. Convergence of the method is assured according to the Weierstrass approximation theorem. The polynomial approximation (algorithm) is very easy to understand, and one can implement this in various fields of study.

2. MATERIAL AND METHODS

2.1. Study area

The Pindrawan tank command area was the area under study (Figure 1); it is situated within 81 °45′–81 °50′ E and 21 °20′–21 °25′ N in the upper Mahanadi River valley (southeastern part) and comes under Raipur district of Chhattisgarh, India. A total of nine villages, namely, Pauni, Amlitalab, Khauna, Deogaon, Bangoli, Dhansuli, Kurra, Baraonda, and Nilja, falls under the study area, which has a tropical wet and dry climate. The temperature in this part of India remains moderate throughout the year. The highest temperatures in the year observed as 48° between March to June. The maximum rainfall recorded is around 325 mm. The average depth of the groundwater table is a minimum of 0.33 m below ground level (bgl) and a maximum of 17.14mgbl.

2.2. Data collection and WQI analysis

The groundwater samples from open and bore wells (37 sites) are collected and the average value is used for drinking and irrigation purposes in the Prindrawan tank area is given in Table 1. The identification of the sampling points is performed

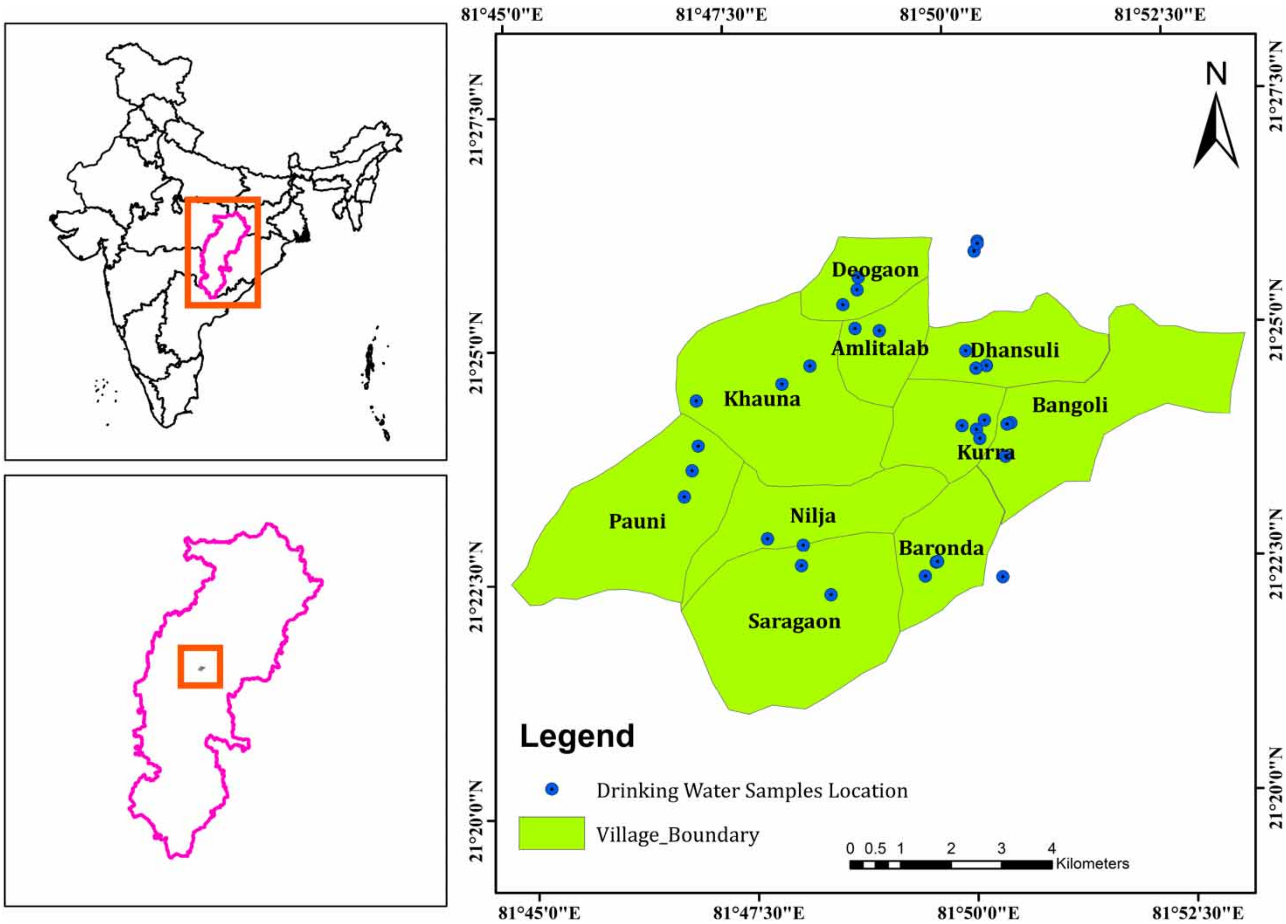


Figure 1 | Map of the study area showing the Pindrawan tank command area's geographical location in Chhattisgarh State, India. The figure shows the location of the study area at the country and state levels, as well as the village boundaries that are under the Pindrawan tank command area with drinking water sample locations (blue color points).

Table 1 | Location of ground water samples

Sample No.	Lat	Long	Sample No.	Lat	Long	Sample No.	Lat	Long
1	81.8282	21.3761	**13**	81.8367	21.3994	**25**	81.8155	21.4273
2	81.8023	21.3764	**14**	81.8373	21.3977	**26**	81.8124	21.4226
3	81.8077	21.371	**15**	81.834	21.4001	**27**	81.8152	21.4252
4	81.7961	21.3815	**16**	81.828	21.376	**28**	81.8584	21.4041
5	81.8028	21.3801	**17**	81.8258	21.3736	**29**	81.8377	21.4311
6	81.7961	21.3815	**18**	81.8282	21.3761	**30**	81.8566	21.4033
7	81.8391	21.4107	**19**	81.7824	21.3942	**31**	81.8001	21.4089
8	81.8353	21.4134	**20**	81.7807	21.3896	**32**	81.8426	21.4
9	81.8371	21.4103	**21**	81.7837	21.3985	**33**	81.8405	21.3729
10	81.8383	21.401	**22**	81.7837	21.4066	**34**	81.8384	21.4329
11	81.842	21.3943	**23**	81.8001	21.4089	**35**	81.8384	21.4325
12	81.8433	21.4002	**24**	81.8056	21.4119	**36**	81.819	21.4177
						37	81.8145	21.4183

using topographic sheets and GPS, and the maps are prepared using ArcGIS 10.1. Topographic sheets are utilized for the preparation of the base map and to recognize the general features of the area. GPS technique is utilized to identify the geographic position of each sampling point. The study area is situated in industrial zone where mining activity is very active like coal, limestone, quarries. Because of these, pH parameter is selected for analysis. Along with this, as per literature fluoride and sulphate is very high i.e., above permissible limit and such contaminated groundwater is not good for human being. That's why fluoride ad sulphate is selected as parameters. The collected groundwater samples are investigated for the concentration of three parameters such as pH, sulphate (SO_4), and fluoride (F) only as per the specification of Federation and American Public Health Association (2005). pH of the collected samples is measured in the field itself using pH meter. The pH determination is usually done by electrometric method, which is the most accurate one, and free from interferences. Turbidimetric method is used for the determination of sulphate ions. Sulphate ion (SO4–) is precipitated in an acetic acid medium with Barium chloride (BaCl2) so as to form Barium sulphate (BaSO4) crystals of uniform size. Light absorbance of the BaSO4 suspension is measured by a photometer or the scattering of light by Nephelometer. The fluoride concentration is analyzed based on the selective electrode method. When the fluoride electrode is dipped in sample whose concentration is to be measured, a potential is established by the presence of fluoride ions by any modern pH meter having an expanded millivolt scale. The fluoride ion selective electrode can be used to measure the activity or concentration of fluoride in aqueous sample by use of an appropriate calibration curve. However, fluoride activity depends on the total ionic strength of the sample. During the analysis, prescribed safety measures are followed. The latitude and longitude values of sampling stations range from 81 °78′ E to 81 °86′ E and 21 °37′ N to 21 °43′ N respectively.

The concentration of the parameters is compared with the acceptable limits prescribed by WHO (2012) and (BIS (IS 10500) 2012). The observed water quality parameters are finally integrated into a combined single parameter referred to as WQI. The WQI in the present study was calculated using the weighted arithmetic index method (Brown *et al.* 1972).

Relative weight (W_i) of each parameter can be computed using Equation (1):

$$W_i = \frac{w_i}{\sum_{i=1}^{n} w_i} \tag{1}$$

where, n represents the number of parameters considered for the groundwater quality assessment. Similarly, quality rating (q_i) for each parameter is calculated as presented in Equation (2).

$$q_i = \left(\frac{C_i}{S_i}\right) \times 100 \tag{2}$$

Table 2 | Details of apparatus used for estimation physicochemical parameters

Sn. No.	Instrument	Manufacturer Name and Model
1	pH meter	Systronics Model: μ Controller Based pH system Type 362
2	EC meter	Systronics Model: Conductivity TDS meter 308
3	Spectrophotometer	Hi Tech, Double Beam Spectrophotometer Model: 3375
4	Flame Photometer	Systronics Model: Flame Compressor 120 (uC) [FPM Compressor 126, Systronics]
5	Kjeldahl Distillation Unit	KELPLUS Model: Classic – DXVA
6	Atomic Absorption Spectrophotometer	ECIL (Electronics Corporation of India Limited) Model: AAS
7	Electrode	Glass and Platinum combined electrode

where, C_i represents the concentration of i^{th} parameter in a specific sample and S_i is the respective permissible standards. Finally, WQI is calculated from Equation (3)

$$WQI = \frac{\sum_{i=1}^{i=n} W_i \times q_i}{\sum_{i=1}^{i=n} W_i} \tag{3}$$

Based on calculated WQI values, the quality of the groundwater for drinking purposes can be classified in to five categories i.e., Excellent water quality (WQI: 0–50), Good water quality (WQI:50–100), Poor water quality (WQI:100–200), Very Poor water quality (200–300), Unfit for drinking (>300).

Finally, the outcomes from the analytical study are taken to the GIS for the preparation of spatial distribution maps. The IDW interpolation method was used from Geospatial analysis tools.

2.3. Mathematical model

In this present study the Weierstrass's polynomial approximation theorem in finite domain is adopted (Schep 2007). For example, the contaminant concentration data for wells, and bore wells at different points in certain finite region was found. Let us assume that we are working for a specific latitude and longitude (p, q) in the very beginning of the process author shift the origin to that specific point. Let $C(x, y)$ be a continuous function in a finite domain $[a_1, b_1] \times [d_1, e_1]$ for a fixed time $t = t_0$ then $C(x, y)$ can be approximated by a polynomial$P(x, y)$ in the domain $[a_1, b_1] \times [d_1, e_1]$.

Where $P(x, y) = \sum_{i=0}^{n} k_i x^i \left(\sum_{j=0}^{n} y^{n-j}\right)$.

For the n finite set of values (C_i, x_i, y_i) we determined n linear equations with n unknowns. By solving these equations, the polynomial $P(x, y)$ is obtained. So, for a certain domain of interest (i.e. specified region) author can assume that various parameters of the groundwater contaminant can be obtained mathematically in from of polynomial. So, by using very less

Table 3 | Comparison of chemical parameters with prescribed standards

Parameter	Experimentally Obtained Range of Concentration in the Collected Samples	Permissible Limits	Percentage of Samples Exceeding Permissible Limits	Undesirable Effect
pH	7.26–8.59	6.5 to 8.5	2.70	Irritation in eyes, skin, and mucous membranes; skin disorders
Sulfate (mg/L)	25–50	200	0	Laxative effect
Fluoride (mg/L)	0.25–0.84	1	0	Mottling of teeth, deformation of bones

number of data along with longitudinal and latitudinal value author can able to predict the amount of the harmful elements throughout the region by putting the latitudinal and longitudinal value. The present problem has been solved by using the MATLAB software. In this present scenario author considered that there is only one aquifer is used throughout the specific region.

3. RESULT AND DISCUSSION

3.1. Water quality index analysis of the field-based samples

The concentration, distribution, and impact of different physicochemical parameters observed from water samples collected from the Pindarwan tank area are discussed in this section. The details of apparatus used for measuring the parameters are

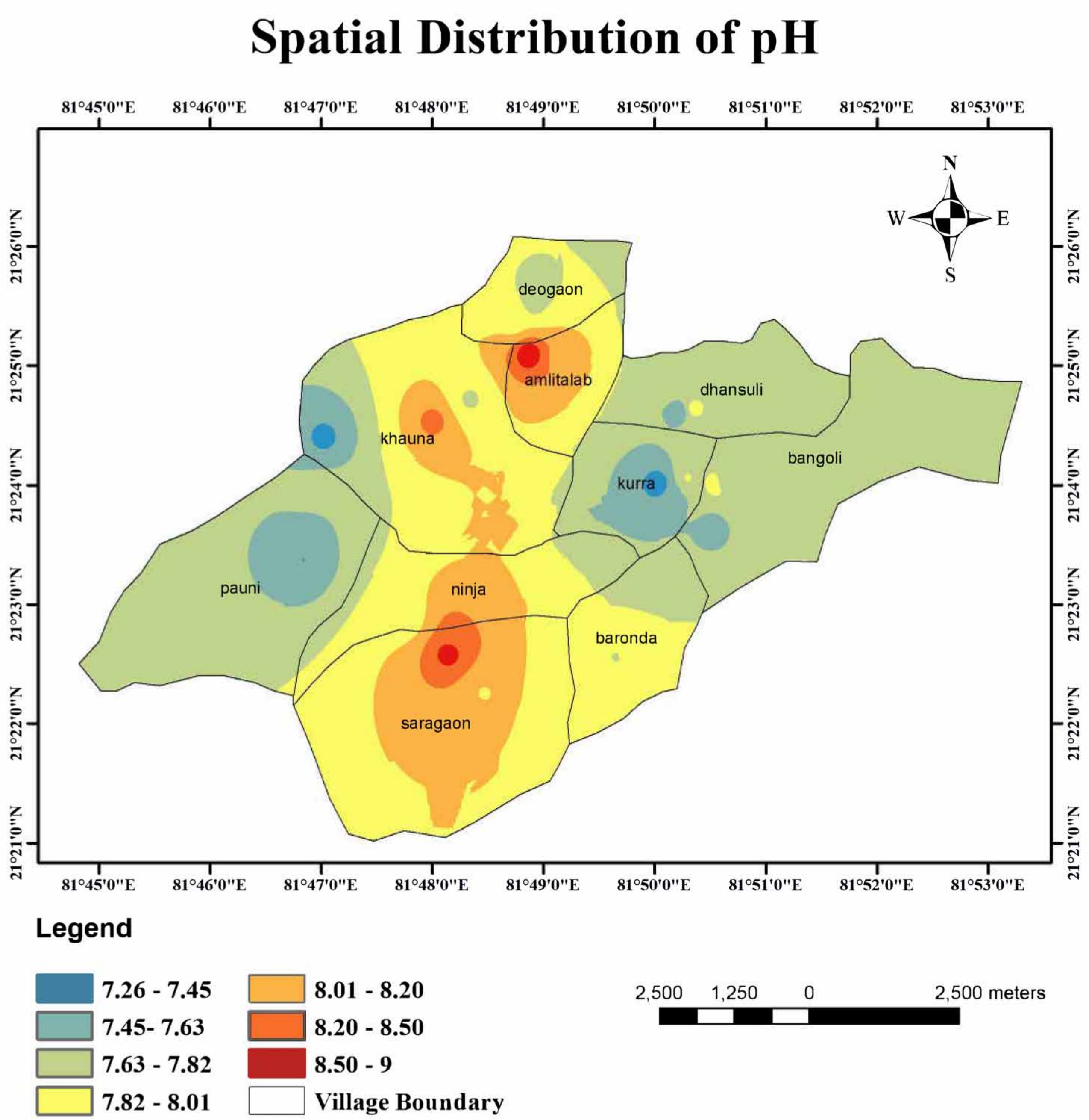


Figure 2 | Spatial distribution of the pH (Source: Agrawal *et al*. 2021b).

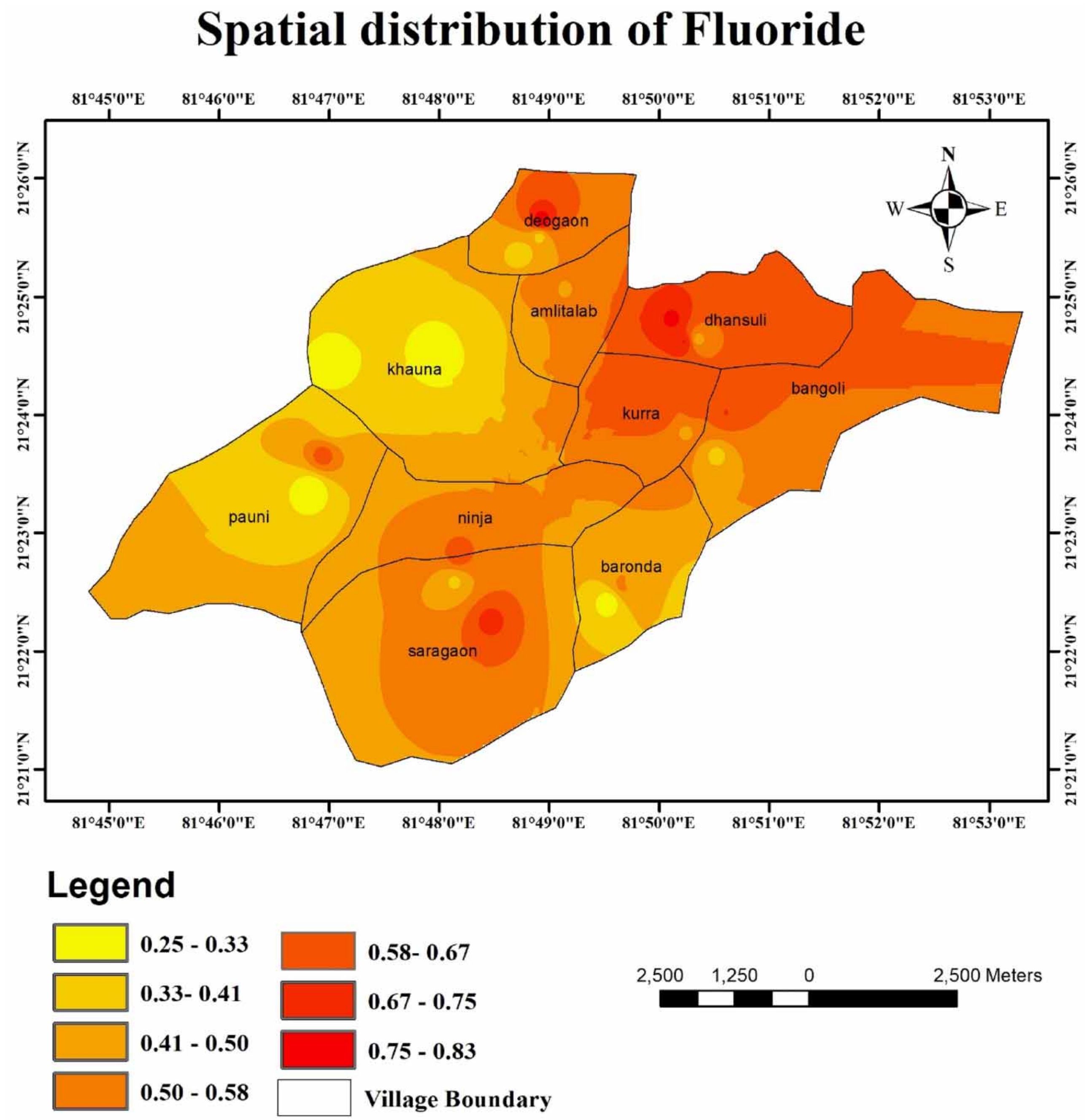


Figure 3 | Spatial distribution of the Fluoride (Source: Agrawal *et al*. 2021b).

provided in Table 2. The ranges of concentrations observed for various parameters and the percentages of total samples exceeding the prescribed limit are presented in Table 3, along with their undesirable effect on groundwater quality and human physiology. This section provides an overview of the spatial distribution of the physicochemical parameters of pH, Fluoride and Sulphate that were measured in the Pindarwan tank area is explained in Figures 2–4. Out of 37 samples, 32.43% of the samples had excellent water quality, 43.24% of the samples had good water quality, 21.62% of the samples had poor water quality, and 2.71% of the samples had very poor water quality. None of the samples fall under Unfit for drinking category. The areas corresponding to these WQI values are presented in Figure 5.

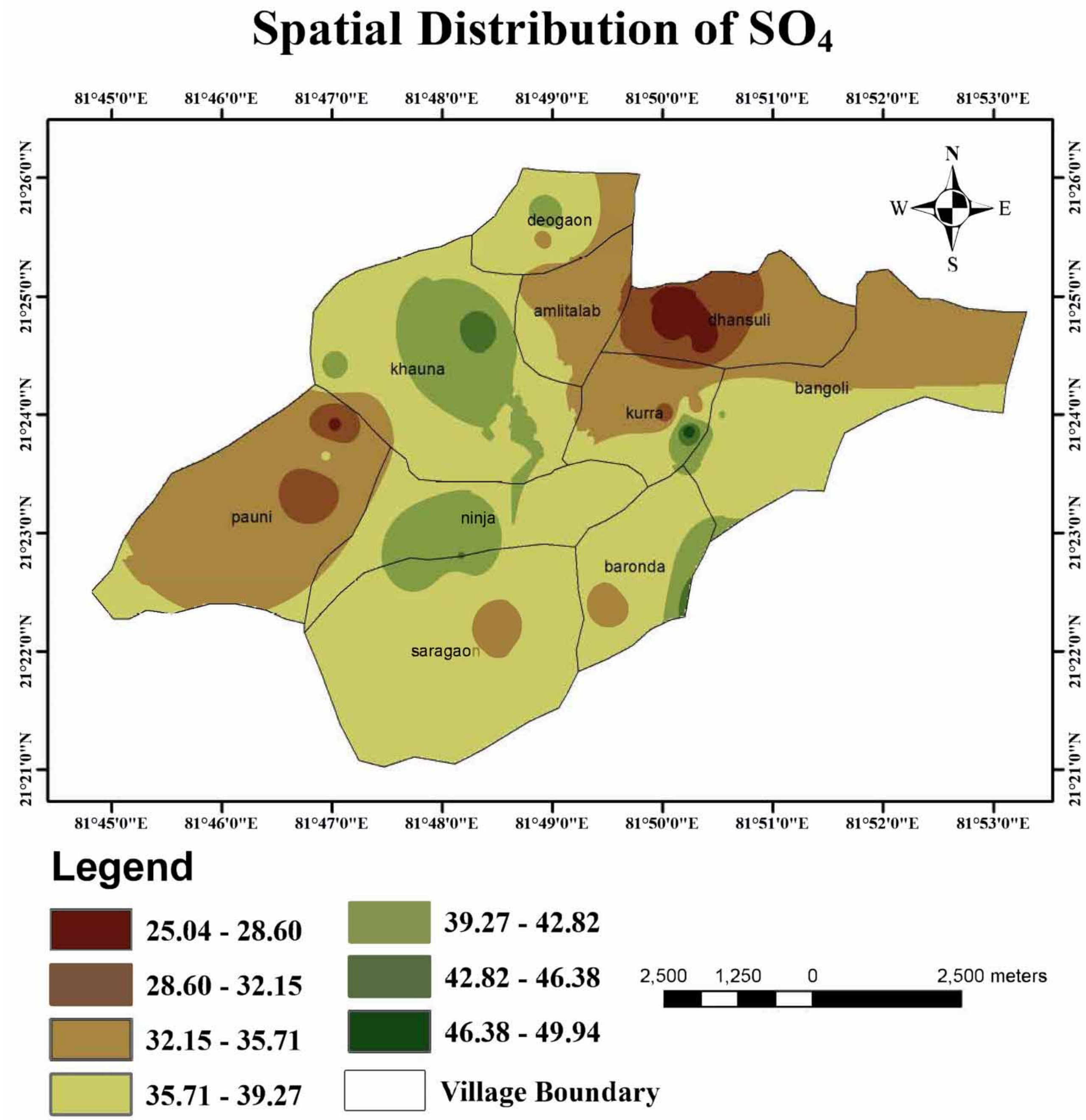


Figure 4 | Spatial distribution of the Sulphate (Source: Agrawal *et al*. 2021b).

For mathematical model, authors used the following data set to obtain the graphical representation of the pH, WQI, Fluoride and Sulphate distribution throughout the domain as given in Table 4.

According to our consideration author shift the origin to (81,21) and then approximate the polynomial. In the Table 1 other rows indicate the concentration of the respective physico-chemical parameters for respective samples. The obtained results or the polynomial for pH, WQI, Fluoride and Sulphate are shown by the graph and in the next section result will be validated with the additional data and the error will be calculated.

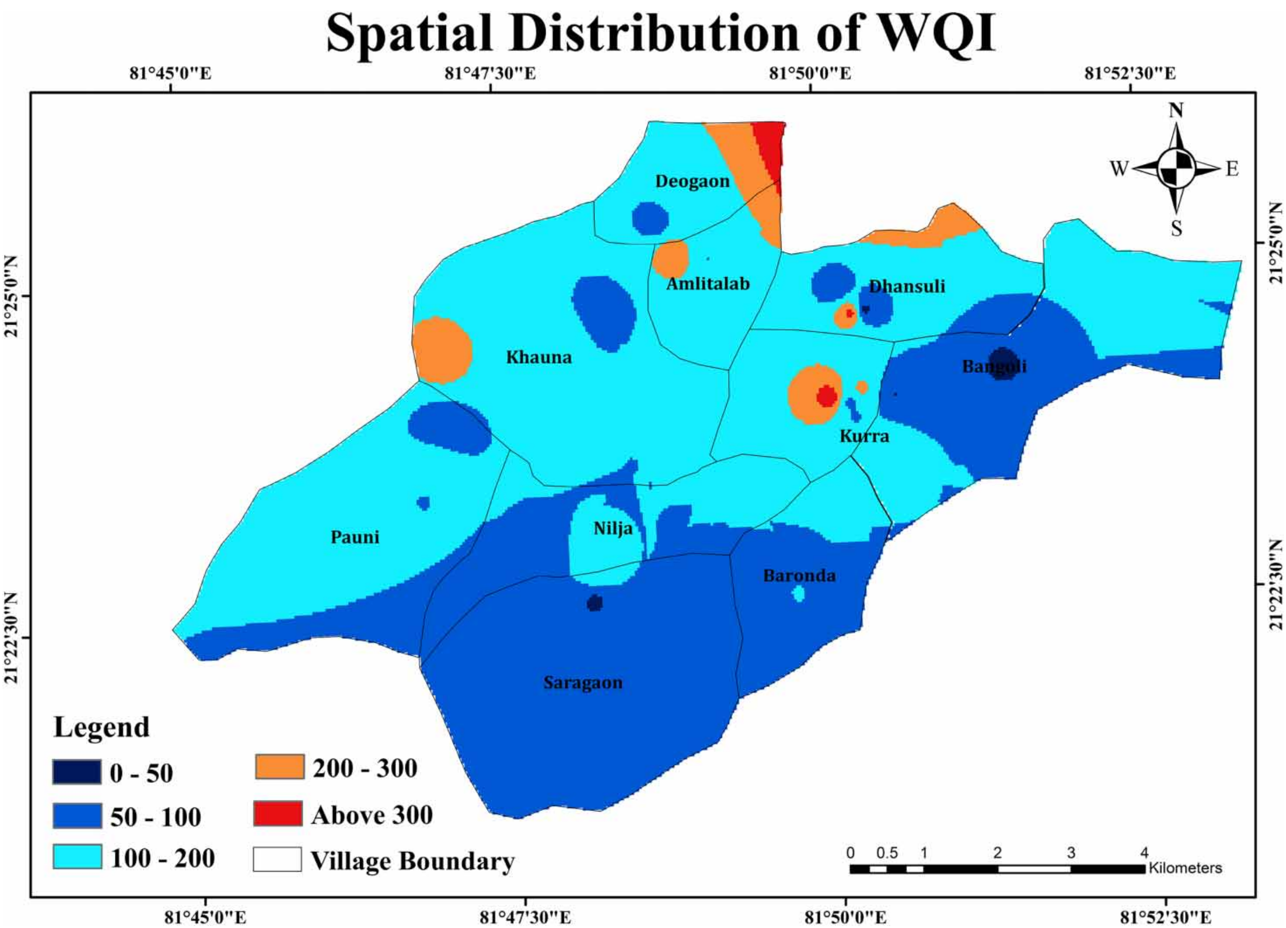


Figure 5 | Spatial distribution of the WQI.

Table 4 | Data set consider for various parameters like pH, WQI, Fluoride and Sulphate

Places	Nilja Bore, c 81.79612/ 21.38146	Saragaon Bore, b 81.80772/ 21.37098	Nilja Bore, c 81.79612/ 21.38146	Dhansuli Bore, c 81.83913/ 21.41065	Dhansuli Bore, b 81.83532/ 21.41343	Bangoli Bore, c 81.84197/ 21.39433	Pavni Bore, b 81.78066/ 21.38957	Barroda Bore, b2 81.82575/ 21.37362	Pavni Bore, c 81.78371/ 21.39852	Khona Bore, b 81.78372/ 21.40658
pH	7.79	8.01	7.87	7.91	7.7	7.59	7.45	7.89	7.75	7.41
WQI	67.43	71.00	87.27	41.30	54.89	127.80	99.30	60.16	58.51	183.29
Fluoride	0.7	0.8	0.54	0.46	0.78	0.38	0.25	0.26	0.36	0.29
Sulphate	34	28	42	26	25	38	29	34	28	40

Table 5 | Validation of the result with pH parameter

Places	Khona Bore, c 81.80561/ 21.41194	Nilja Talab, a 81.80284/ 21.38006	Pavni Pond, a 81.78237/ 21.39418	Saragaon Bore, c 81.80234/ 21.37644	Barroda Bore, b1 81.82796/ 21.37603
pH (Given in Data set)	7.8	8.23	7.6	8.47	7.64
pH (Calculated)	8.56	7.4	7.67	7.65	7.18
Relative Error	0.09	0.1	0.01	0.09	0.06

Table 6 | Validation of the result with Fluoride parameter

Places	Khona Bore, c 81.80561/ 21.41194	Barroda Pond, a 81.82821/ 21.37609	Pavni Pond, a 81.78237/ 21.39418	Saragaon Bore, c 81.80234/ 21.37644	Pavni Bore, b 81.78066/ 21.38957
Fluoride (Given in Data set)	0.024	0.203	0.227	≈0	≈0
Fluoride (Calculated)	0	0.300	0.37	0	0.009(≈0)
Relative Error	1	0.47	0.62	0	0

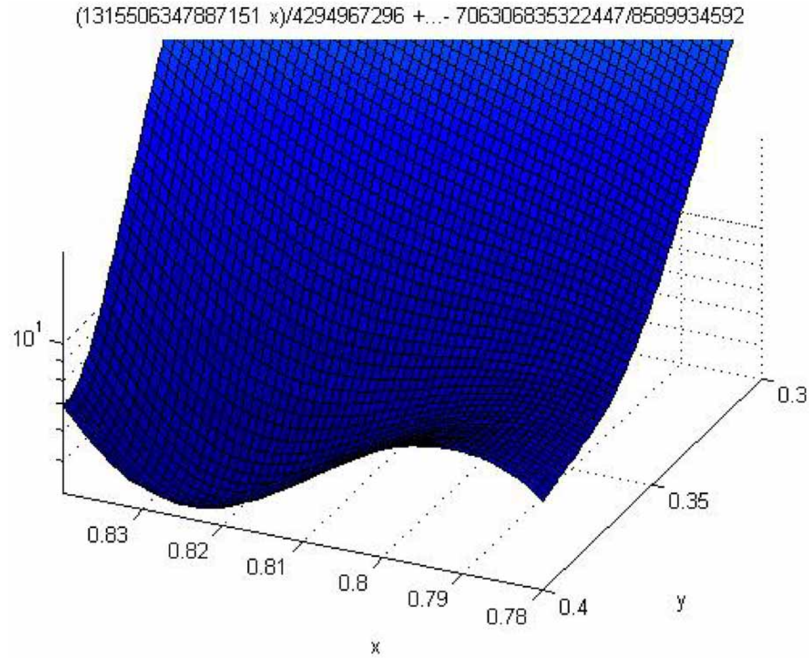


Figure 6 | Observed pH Value for the Domain.

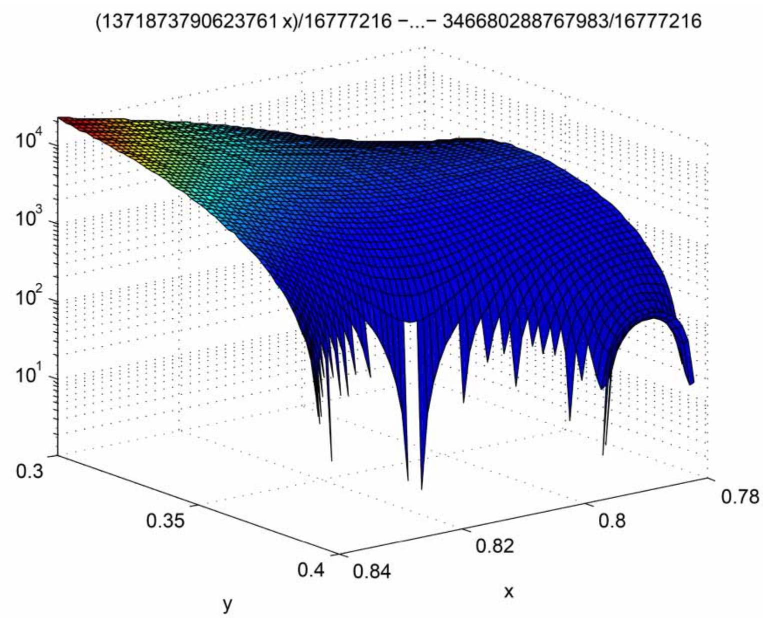


Figure 7 | Observed WQI Value for the Domain.

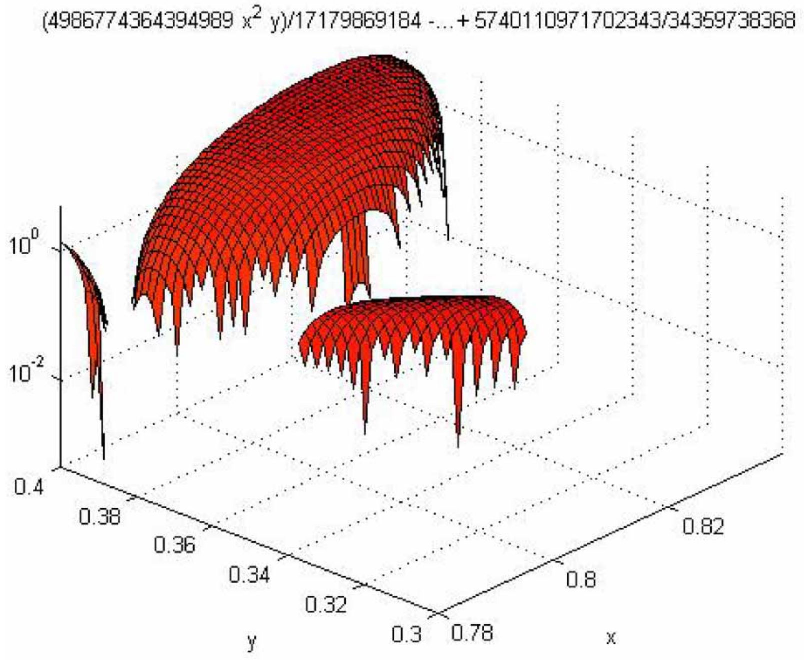


Figure 8 | Observed Fluoride Value for the Domain.

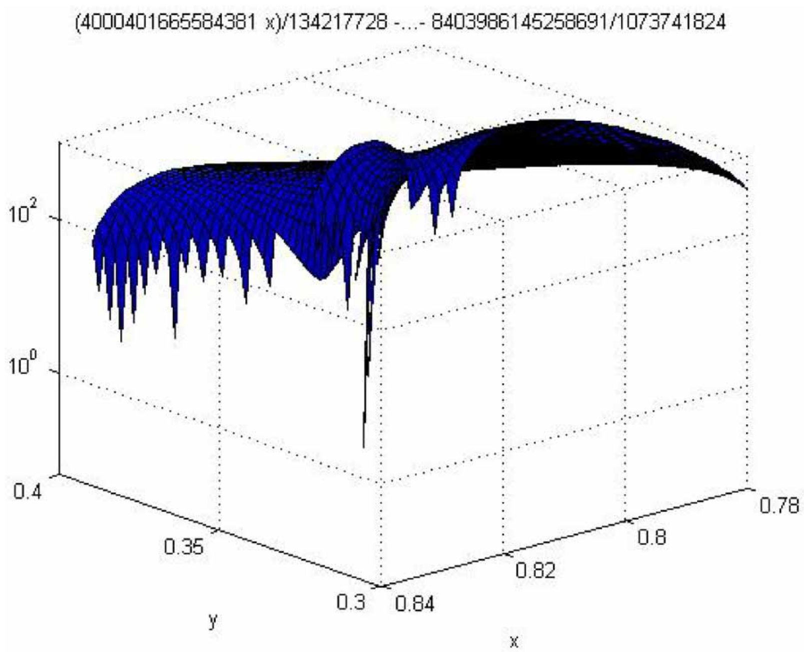


Figure 9 | Observed SO_4 Value for the Domain.

3.2. Validation with field data

In this section authors want to verify the obtained result with unused data. Authors are going to validate the result with one of the presented contaminants if our results match with the real data then we can say that the used methodology is better to use. To validate the result authors, consider pH level and Fluoride as shown in Tables 5 and 6 respectively.

So, the average relative error is 0.07 (pH) and 0.04 (Fluoride), hence the percentage error is 7% (pH) and 40% (Fluoride). So, it is clear that the methodology we have used is accurate. Hence, polynomial approximation can be one of the replacements for this type of problem.

4. CONCLUSION

The process of WQI estimation is often associated with handling large quantities of identical data. This can create significant confusion during the calculation process and make decision making difficult. Using this simple polynomial approximation although powerful methodology, groundwater quality prediction can be done more accurately. The major two benefits of this method are: 1. Easy to understand (anyone can be able to use the method.). 2. Requirement of less data (Small set of data is enough to determine the polynomial.). Using the polynomial approximation method one can easily able to obtain the WQI index of his position and able to take decision that stakeholder may consume the water or not? The error is found 7% approximately. which is significantly small. So, the proposed method can be very effective and useful. This polynomial approximation method can also be used as the substitute of inverse modeling to determine the location of the source in three-dimension system. Depending upon the availability of data, in future analysis more numbers of parameters will be utilized under different weather conditions.

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DATA AVAILABILITY STATEMENT

Data cannot be made publicly available; readers should contact the corresponding author for details.

CONFLICT OF INTEREST STATEMENT

The authors declare there is no conflict.

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