



Research article

Geographical analysis of fluoride and nitrate and its probabilistic health risk assessment utilizing Monte Carlo simulation and GIS in potable water in rural areas of Mathura region, Uttar Pradesh, northern India

Shahjad Ali^{a,*}, Salman Ahmad^b, Mohammad Usama^c, Raisul Islam^d, Azhar Shadab^e, Rajesh Kumar Deolia^f, Jitendra Kumar^g, Ayoob Rastegar^h, Ali Akbar Mohammadi^{i,j,**}, Shadab Khurshid^b, Vahide Oskoei^k, Seyed Alireza Nazari^l

^a Department of Environmental Science, Sharda School of Smart Agriculture, Sharda University Agra, Keetham, Agra, 282007 India

^b Interdisciplinary Department of Remote Sensing and GIS Applications, Aligarh Muslim University, Aligarh, India

^c Department of Environmental Science, Integral University, Lucknow, India

^d Department of Civil Engineering, GLA University Mathura, India

^e Department of Electronics and Communication Engineering G. L. Bajaj Institute of Technology and Management, Greater Noida, Uttar Pradesh, 201306, India

^f Department of Applied Science (Mathematics), G.L. Bajaj Group of Institutions, Mathura, India

^g Department of Mathematics and Computing, Madhav Institute of Technology and Science, Gwalior, India

^h Department of Environmental Health, School of Health and Non-Communicable Diseases Research Center, Sabzevar University of Medical Sciences, Sabzevar, Iran

ⁱ Department of Environmental Health Engineering, Neyshabur University of Medical Sciences, Neyshabur, Iran

^j Workplace Health Research Center, Neyshabur University of Medical Sciences, Neyshabur, Iran

^k School of Life and Environmental Science, Deakin University, Geelong, Australia

^l Medical Nanotechnology Tehran University of Medical Sciences, School of Advanced Technologies in Medicine. Tehran, Iran

ARTICLE INFO

Keywords:

Contamination
Fluoride
Health risk assessment
Mathura rural area
Monte Carlo simulation
Nitrate
Probabilistic

ABSTRACT

Human health is being increasingly exposed to fluoride and nitrate ingestion globally due to anthropogenic alternations in groundwater resources. In the present research work, a hazard quotient (HQ), Monte Carlo simulation (MCS), and geographic information systems (GIS) have been used to estimate the non-carcinogenic health risk of nitrate and fluoride in vulnerable adults, teenagers, and children living in far-flung areas of Uttar Pradesh, Northern India. About 110 samples from some nearby populations were collected and analyzed for nitrates by ion chromatography and fluoride by a fluoride-selective electrode. The results indicated that the concentrations of fluoride and nitrate in the sampling areas ranged from 0.21 to 1.71 mg/L and 0.4–183.54 mg/L, respectively, with mean concentrations of about 1.20 mg/L and 51.52 mg/L for fluoride and nitrate, respectively. The results indicated that 27.27 % of the fluoride samples (27 out of 110) and 45.45 % of the nitrate samples (44 out of 110) were above the standard limits set by WHO. The calculated average HQ values fluoride and Nitrate for children, teenagers and adults were 1.88, 0.98, 0.90 and 3.02, 1.57, 1.45 respectively The 95th percentile HQ values for fluoride

* Corresponding author. Department of Environmental Science, Sharda School of Smart Agriculture, Sharda University Agra, Keetham, Agra, 282007 India.

** Corresponding author. Department of Environmental Health Engineering, Neyshabur University of Medical Sciences, Neyshabur, Iran.

E-mail addresses: shahjadali@agra.sharda.ac.in (S. Ali), mohammadia3@nums.ac.ir (A.A. Mohammadi).

<https://doi.org/10.1016/j.heliyon.2024.e37250>

Received 18 June 2024; Received in revised form 28 August 2024; Accepted 29 August 2024

Available online 30 August 2024

2405-8440/© 2024 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY-NC license (<http://creativecommons.org/licenses/by-nc/4.0/>).

were 2.87 for children and 1.03 for adults, while those for nitrate were 4.10 for children and 1.98 for adults. Results of the health risk assessment show that there is a high potential for both non-carcinogenic and cancer risks from fluoride and nitrate through the consumption of groundwater. The Monte Carlo simulation showed the uncertainties and increased risks for children; therefore, one can infer that rural groundwater of the Mathura region, Uttar Pradesh, India, must be treated to make it potable for consumption.

1. Introduction

Groundwater (GW) is the major source of potable water for municipal, agricultural, and industrial uses. But, nowadays, its quality is continuously deteriorating due to demographic burdens and various industrial activities [1–4]. One of the crucial elements in assessing whether groundwater is suitable for drinking water is the qualitative and quantitative evaluation of the resource [5,6].

Many countries, particularly Iran and India, rely on GW as a potable water source, since it is among the most significant water resources in the world. However, due to several factors, including the growth of agriculture and industry, the development of urbanization, and drought, GW is polluted by a variety of water pollutants [7–10]. In today's world, people mostly use contaminated water which leads to the spread of several water-borne diseases [11–14]. But there are a lot of people working hard for the government and nongovernmental organization (NGOs) to make sure that everyone has access to clean water. The contaminants like dissolved solids, heavy metals, suspended particles, pesticides, and emerging contaminants (inorganic and organic chemicals) have been reported in water, causing a variety of health problems [13–17]. The major issue nowadays is the presence of fluoride (F^-) in drinking water. Its concentration in potable water may be both a boon and bane, as it is suitable at 1.5 mg/L, but the higher concentration of fluoride (>1.5 mg/L) is harmful to human health [18–20]. About 200 million people across 25 nations are using fluoride-contaminated potable water [21,22]. A high fluoride concentration in GW may be caused by natural or anthropogenic dissolution of fluoride-enriched granitic rocks [23]. Some rocks have fluorine-rich minerals, like biotite, cryolite, fluorapatite, fluorite, hornblende, muscovite, topaz. Some of these rocks can get easily dissolved in GW and release F^- ions [24]. The anthropogenic sources have increased the F^- ions in GW through industrial waste, coal combustion, and overuse of fertilizers in agricultural land. The geogenic sources of fluoride include ion exchange, rock-water morphology, rock nature, and calcite precipitation [25–27]. Continuous exposure to fluoride (>1.5 mg/L) causes severe health issues like fluorosis i.e. bone dental, and skeletal fluorosis, and bone cancer, impotency [28–33]. According to certain research, consuming nitrates (NO_3^-) through food and drink can lead to nervous system abnormalities, birth malformations, or low birth weight in infants [34–36]. There have been cases of Methemoglobin, gastrointestinal problems, and stomach cancer in the Fars area of Iran [9,37,38]. Monte Carlo simulations are utilized in the present research work to evaluate the concentration of fluoride and nitrate contamination in groundwater through exposure [39]. According to a research study, a notable correlation was observed between GW and F^- concentration [40]. In GW, fluoride is mainly derived from surface water (river, pond, and lake). The main reason for fluoride importation to the GW is the infiltration of irrigation canals and rivers. Wastewater treatment plants and agricultural runoff water polluted by chemical fertilizer discharge are the main contributors to nitrate levels in groundwater [41]. The high fluoride and nitrate concentrations in the rural Mathura area may likely be controlled by some unique geology of the area leading to their higher concentration [39,41]. Added to this, agricultural and urbanization anthropogenic activities may also aggravate the contamination. Overall, natural and anthropogenic factors make groundwater unsatisfactory for consumption and require efficient treatment solutions [41].

Despite the fact that much research has been done with regard to fluoride and nitrate contamination in groundwater, a few critical gaps remain to be addressed [41]. There are hardly any regional studies that provide complete coverage for all villages in the Mathura region [41]. The correlation of land use patterns and contamination levels has hardly been looked into. There is also a striking shortage of studies using Monte Carlo simulation for health risk assessment model based on demographic and environmental factors [39]. The long-term health effects in different demographic groups are also not considered adequately in most of the studies [32]. Standardized protocols for Monte Carlo simulation in health risk assessments are lacking, and sensitivity analysis to identify key risk factors is rarely conducted. Few comparative studies have shown the effectiveness of Monte Carlo simulation over traditional methods [33,42]. These gaps point to the need for more localized, interdisciplinary, technically integrated studies to increase understanding and mitigation of health risks due to fluoride and nitrate contamination in rural areas [41]. The main goals of the present research work are (i) to collect water samples from nearby villages in the rural area of Mathura region, Uttar Pradesh (UP), India. The sample collection focuses on examining the presence of nitrate and fluoride in the water and its comparison to the national and international standards (ii) to use ArcGIS software to assess the possible health risks of nitrate exposure from contaminated drinking water in three targeted groups i.e children, teenagers and adults (iii) to determine the quantitative uncertainties and critical input parameters during the risk assessment process (iv) this research work is to examine the origins, dispersion, and dynamics of elevated levels of fluoride and nitrate in rural Mathura, UP, India. The present study intends to examine the origins, dispersion, and genesis of elevated concentrations of F^- and NO_3^- in rural Mathura, Uttar Pradesh, India. The findings of this research will help with the suitable corrective measures, such as granting access to centralized and substitute sources of supply of good water.

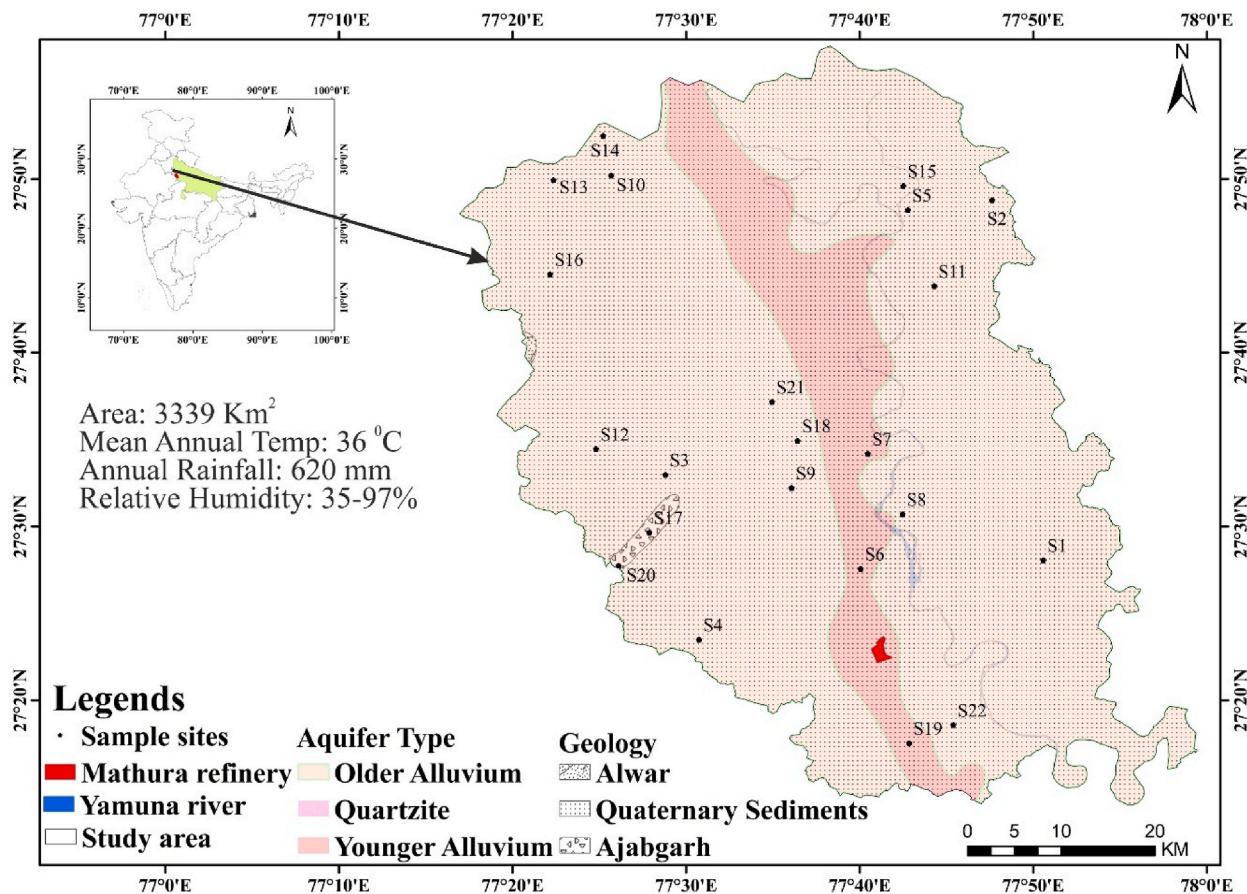


Fig. 1. Locations of rural area of Mathura, Uttar Pradesh, India.

2. Materials and techniques

2.1. Study areas

The region of Mathura is located in UP's western region (Fig. 1). It is situated about 50 km to the north of Agra. For Hindus, Mathura is a sacred place because it is thought to be the birthplace of Krishna. Approximately 2.5 billion people call this place home, and it is the largest district in Uttar Pradesh, India. The area under investigation spans approximately 3339 km² and is located between longitudes 77° 17' and 78° 12' and latitudes 27° 14' and 27° 17'.

2.2. Examination and assessment of the collected samples

Underground water samples were gathered from various nearby sighted villages (110) having contaminated water to comprehend the study from March 2019 to February 2020, as depicted in map Fig. 1. Ionic chromatography and a fluoride selective electrode were employed for the concentration analysis of nitrate and fluoride, respectively [43]. The Fig. 2 depicted the flowchart of scientific methodology which includes the complete process of the sample analysis techniques.

2.3. Human health risk assessment (HRA)

F⁻ and NO₃⁻ concentrations in GW was estimated using the US (USEPA) 1989 model. F⁻ and NO₃⁻, two contaminants in ground-water, were evaluated for their non-carcinogenic and carcinogenic potential using this model. It is based on Eqs. (1) and (2). Table 1 lists the characteristics that were utilized to calculate the estimated daily intake (EDI) [39,44].

$$EDI_{mg} = \frac{C * IR * EF * ED}{BW * AT} \quad \text{Eq. (1)}$$

Where,

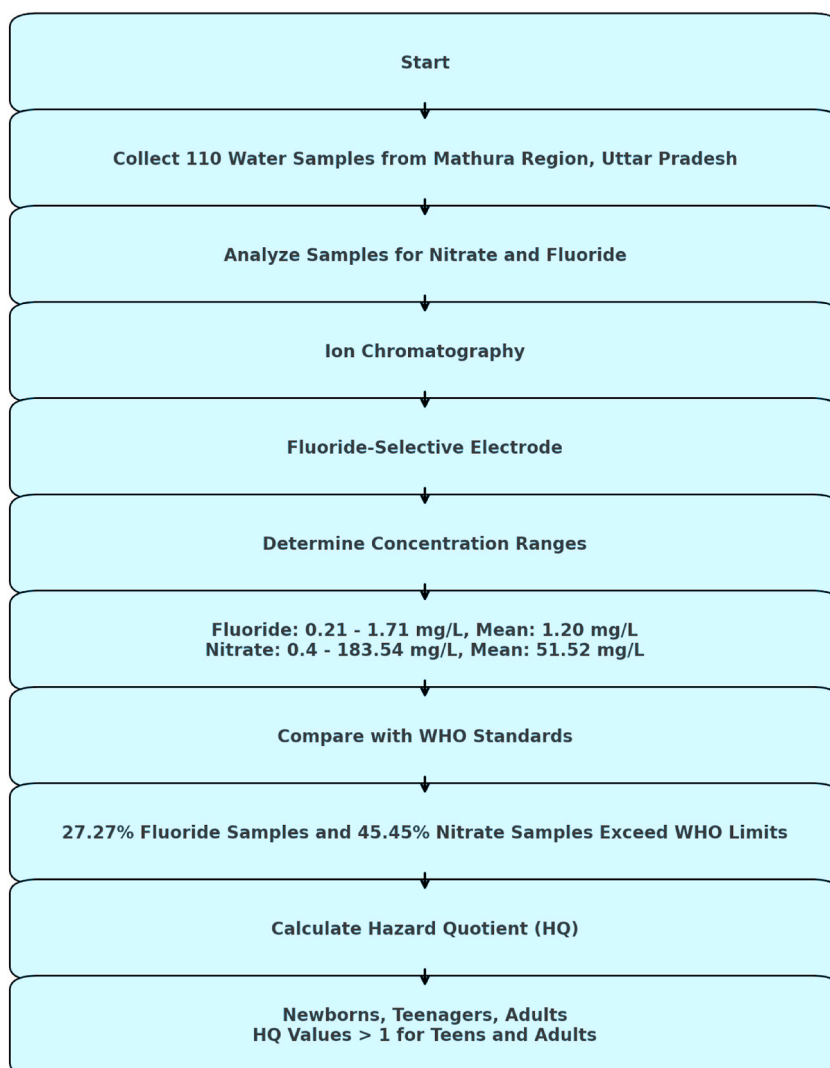


Fig. 2. Flow chart of scientific methodology.

Table 1

Considerations for the health risk method's parameter values [45–47].

Parameters	Symbol	Unit	Children (0–10)	Teenagers (11–20)	Adults (>20)
Average time	AT	Days	EF*ED	EF*ED	EF*ED
Bodyweight	BW	Kg	16	45	62
Exposure duration	ED	Year	4	13	40
Exposure frequency	EF	days/year	345	345	345
Ingestion rate	IR	L/d	1.5	2.2	2.8

EDI_{ing} : Fluoride and nitrate Consumption Per Day (mg/kg/day)

C: Concentrations of fluoride and nitrate concentration (mg/L)

Equation (2) of (HQ) is used to determine the non-carcinogenic and carcinogenic risks associated with fluoride exposure [17,39,47].

$$HQ = \frac{EDI}{Rfd} \quad \text{Equation (2)}$$

The reference dosage (Rfd), which is used to compute risk assessment, approximates the population's daily intake without a significant risk of adverse effects over time. There were Rfd values for F (0.06 mg/kg/d) and NO_3 (1.6 mg/kg/d) in the Integrated Risk

Table 2

The fluoride and nitrate parameters utilized in MCS and the uncertainty analysis [29,33,39,46,47,52,53].

Parameter	Age group			Probability Distribution
	Children	Teenagers	Adults	
Ingestion Rate (L/d)	1.25 ± 0.57	1.58 ± 0.69	1.95 ± 0.64	Normal
Body weight (kg)	16.68 ± 1.48	46.25 ± 1.18	57.03 ± 1.10	Log normal
Exposure Duration (year)	4	13	40	Fixed value
Exposure Frequency (days/year)	Minimum = 185, mode = 345, maximum = 365			Triangular
F ⁻ Oral reference dose (RfD) (mg/kg/day)	0.06			Fixed value
NO ₃ ⁻ Oral reference dose (RfD) (mg/kg/day)	1.6			Fixed value

Table 3

Statically analysis concentrations of fluoride in the rural Mathura, Uttar Pradesh, India.

S.No.	Sampling Locations	Fluoride Levels (mg/L)		Ranges	
		Mean	STDEV	Min	Max
1	Pachawar	0.21	0.09	0.11	0.32
2	Khaeera	1.54	0.12	1.4	1.72
3	Kunjera	1.25	0.11	1.15	1.4
4	Lohariya patti	0.7	0.26	0.4	1.1
5	Sultanpur	0.75	0.14	0.59	0.96
6	Narauli	1.03	0.13	0.86	1.21
7	Vrindavan	1.16	0.14	0.93	1.28
8	Laxminagar	1.71	0.13	1.58	1.9
9	Bati	0.73	0.09	0.64	0.85
10	Kharot	1.45	0.08	1.37	1.56
11	Tainti gaon	1.44	0.10	1.34	1.58
12	Kamar	1.07	0.14	0.9	1.23
13	Dhaigaon	1.65	0.18	1.5	1.94
14	Hetana	1.61	0.10	1.51	1.76
15	Pithora	1.71	0.12	1.55	1.88
16	Gidoh1(Nandgaon)	1.29	0.10	1.18	1.43
17	Goverdhan1	0.85	0.16	0.65	1.08
18	Jait	0.99	0.18	0.82	1.28
19	Jamalpur, Farah	1.35	0.09	1.24	1.45
20	Jatipura	0.91	0.15	0.76	1.14
21	Chaumauha1	1.35	0.11	1.16	1.45
22	Chamarpura(chandrabhan), Farah	1.67	0.18	1.5	1.95

Table 4

Statically analysis concentrations of nitrate in the rural Mathura, Uttar Pradesh, India.

S.No.	Sampling Locations	Nitrate Levels (mg/L)		Ranges	
		Mean	STDEV	Min	Max
1	Pachawar	77.7	9.96	65	92
2	Khaeera	8.7	3.03	5.4	13
3	Kunjera	10.7	1.92	8.5	13
4	Lohariya patti	4.8	2.77	2	9
5	Sultanpur	65	12.83	55	87
6	Narauli	35	7.58	24	43
7	Vrindavan	32	6.52	22	39
8	Laxminagar	2.7	1.04	1.5	4
9	Bati	12.6	2.63	9.5	16
10	Kharot	4.6	1.63	2.8	7
11	Tainti gaon	20	4.53	16	27
12	Kamar	0.4	0.19	0.2	0.7
13	Dhaigaon	47	10.07	36	61
14	Hetana	117	10.49	106	132
15	Pithora	8.8	2.39	6	12
16	Gidoh1(Nandgaon)	110.48	11.20	95	126.4
17	Goverdhan1	62.89	6.19	54	71
18	Jait	95.87	15.72	78	119
19	Jamalpur, Farah	183.54	15.47	164.2	205.5
20	Jatipura	156.53	11.05	144	172.15
21	Chaumauha1	65.09	12.55	52	80
22	Chamarpura(chandrabhan), Farah	11.96	3.42	9	17

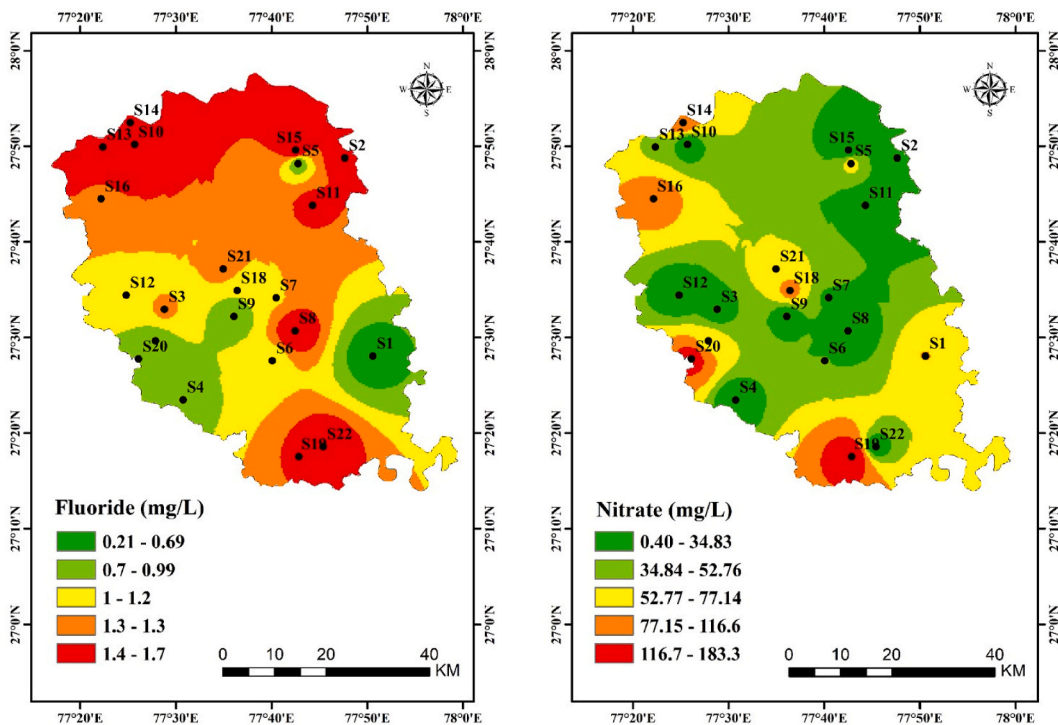


Fig. 3. Regional distribution of F⁻ and NO₃⁻ concentration in rural area of Mathura region, U. P., India.

Table 5

HQ (Fluoride) computation was done using predestinarians in the selected areas of Mathura, Uttar Pradesh, India.

S.No.	Location	HQ (Fluoride)		
		Children	Teenagers	Adults
SN1	Pachawar	0.33	0.17	0.16
SN2	Khaeera	2.41	1.25	1.16
SN3	Kunjera	1.95	1.02	0.94
SN4	Lohariya patti	1.09	0.57	0.53
SN5	Sultanpur	1.17	0.61	0.56
SN6	Narauli	1.61	0.84	0.78
SN7	Vrindavan	1.81	0.95	0.87
SN8	Laxminagar	2.67	1.39	1.29
SN9	Bati	1.14	0.59	0.55
SN10	Kharot	2.27	1.18	1.09
SN11	Tainti gaon	2.25	1.17	1.08
SN12	Kamar	1.67	0.87	0.81
SN13	Dhaigaon	2.58	1.34	1.24
SN14	Hetana	2.52	1.31	1.21
SN15	Pithora	2.67	1.39	1.29
SN16	Gidoh1(Nandgaon)	2.02	1.05	0.97
SN17	Goverdhan1	1.33	0.69	0.64
SN18	Jait	1.55	0.81	0.75
SN19	Jamalpur, Farah	2.11	1.10	1.02
SN20	Jatipura	1.42	0.74	0.68
SN21	Chaumauha1	2.11	1.10	1.02
SN22	Chamarpura(chandrabhan), Farah	2.61	1.36	1.26
	Min	0.33	0.17	0.16
	Max	2.67	1.39	1.29
	Avg	1.88	0.98	0.90

Information System (IRIS) database. The data was obtained from the IRIS of the US Environmental Protection Agency (USEPA). Equation (2) is used to calculate the Hazard Quotient. With concentration levels exceeding the limit and likely having negative impacts on disease and health, HQ1 denotes a non-carcinogenic risk [39,48,49].

Table 6
Predestinarianism has been used to compute HQ (Nitrate) in rural Mathura, Uttar Pradesh, India.

S.No.	Location	HQ (Nitrate)		
		Children	Teenagers	Adults
SN1	Pachawar	4.55	2.37	2.19
SN2	Khaeera	0.51	0.27	0.25
SN3	Kunjera	0.63	0.33	0.3
SN4	Lohariya patti	0.28	0.15	0.14
SN5	Sultanpur	3.81	1.99	1.83
SN6	Narauli	2.05	1.07	0.99
SN7	Vrindavan	1.88	0.98	0.9
SN8	Laxminagar	0.16	0.08	0.08
SN9	Bati	0.74	0.39	0.36
SN10	Kharot	0.27	0.14	0.13
SN11	Tainti gaon	1.17	0.61	0.56
SN12	Kamar	0.02	0.01	0.01
SN13	Dhaigaon	2.75	1.44	1.33
SN14	Hetana	6.86	3.58	3.3
SN15	Pithora	0.52	0.27	0.25
SN16	Gidoh1(Nandgaon)	6.47	3.38	3.12
SN17	Goverdhan1	3.68	1.92	1.78
SN18	Jait	5.62	2.93	2.71
SN19	Jamalpur, Farah	10.75	5.61	5.18
SN20	Jatipura	9.17	4.78	4.42
SN21	Chaumauha1	3.81	1.99	1.84
SN22	Chamarpura(chandrabhan),Farah	0.7	0.37	0.34
	Min	0.02	0.01	0.01
	Max	10.75	5.61	5.18
	Avg	3.02	1.57	1.45

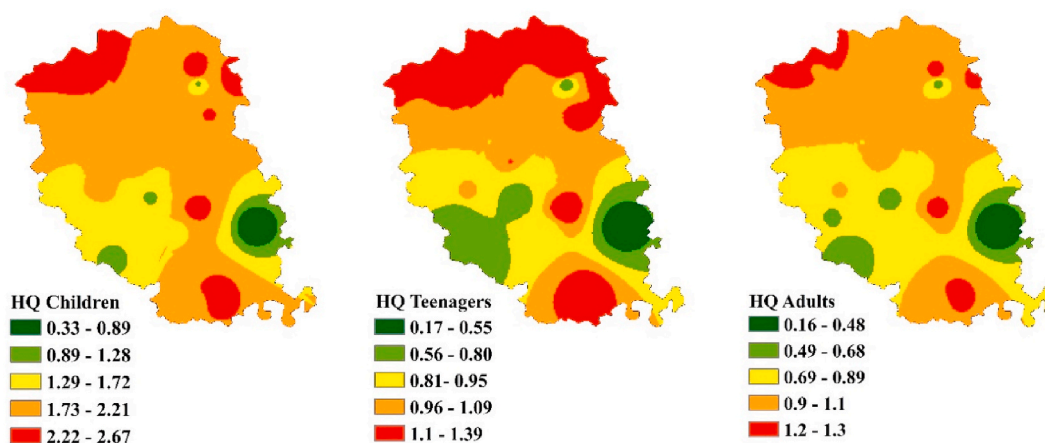


Fig. 4. Regional distribution of HQ (Fluoride) in targeted groups: Children, Teens and Adults in study area of Mathura region, U. P, India.

2.4. Monte Carlo simulation (MCS) & sensitivity analysis (SA)

Monte-Carlo simulation (MCS) was used to estimate the potential danger to human risk by taking into consideration the unpredictability and uncertainty associated with numerous parameters (Table 2). The sensitivity analysis has been conducted through 10,000 iterations using Oracle Crystal Ball (version 11.1.34190) software for MCS. From their fitted distribution, MCS selected the parameter values that allowed them to assess exposure risk and point value [50]. Variations in MCS output, which might be attributed to changes in the input data, were examined using sensitivity analysis (SA) [51]. The used probability distribution functions in the SA and MCS calculate according to USEPA [44].

3. Result and discussion

3.1. Fluoride and nitrate distribution in rural Mathura, Uttar Pradesh, India

Water samples taken from remote areas in the Mathura region showed nitrate concentrations ranging from 0.21 to 1.71 mg/L and

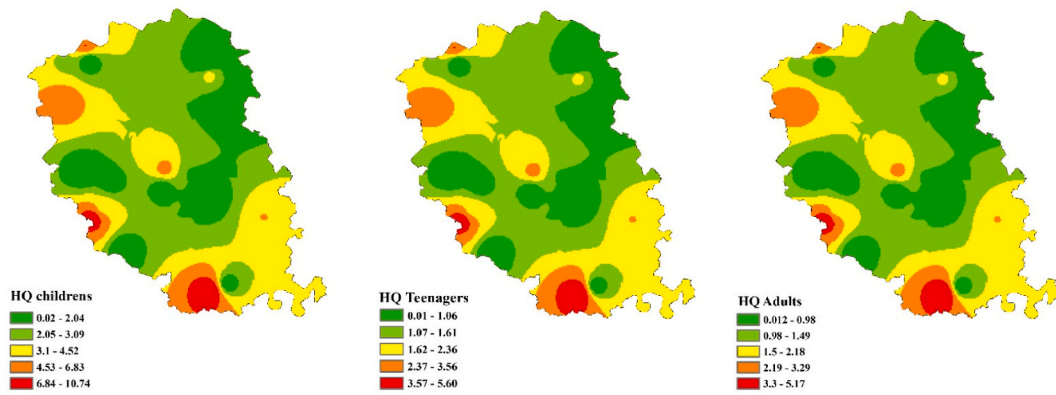


Fig. 5. Regional distribution of HQ (Nitrate) in targeted groups: Children, Teens, and Adults in the study area of Mathura region, U. P, India.

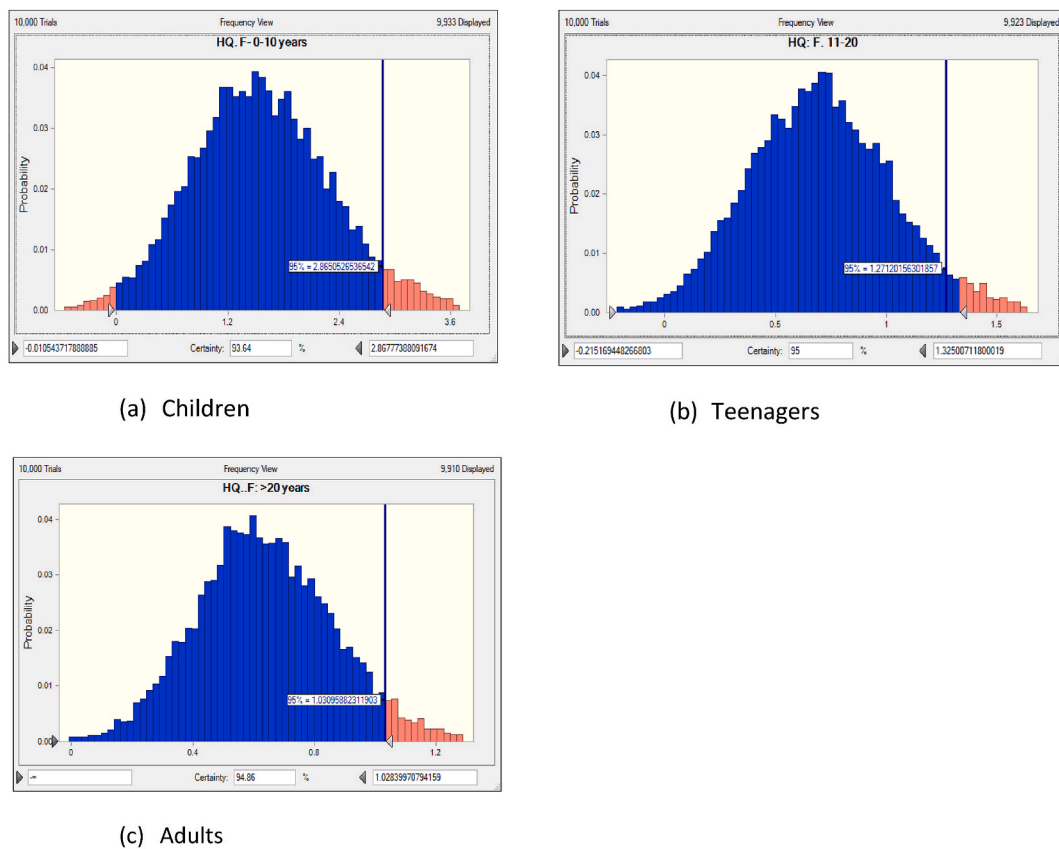


Fig. 6. a, b, c. Bar graphs displaying the results of Fluoride HQ's uncertainty analysis in Children, Teenagers, and Adults groups for the remote areas of the Mathura region, U.P, India.

fluoride values from 0.4 to 183.54 mg/L. As shown in Tables 3 and 4. The fluoride content in the groundwater sample was 1.71 mg/L in Laxminagar and 0.21 mg/L in Pachawar. The nitrate concentration was 183.54 mg/L in Jamalpur and 0.4 mg/L in Kamar, by the same groundwater sample. The WHO (2011) acceptable limit for drinking water was found to be exceeded by 1.51 mg/L and 50 mg/L [18].

Fig. 3 shows F and NO₃ distribution in the sampling locations and five samples were taken from each location. The zoning calculations, Monte Carlo simulations, and risk assessment analyses were based on the average values of these five points. The analysis conducted by S. Ahmed et al. (2020) on all the collected samples within the study area shows that the concentrations of fluoride and nitrate are between 0.03 and 1.71 mg/L and 0.41–191 mg/L, respectively [41]. The above study shows that a large number of villages did not meet the required WHO standards [18].

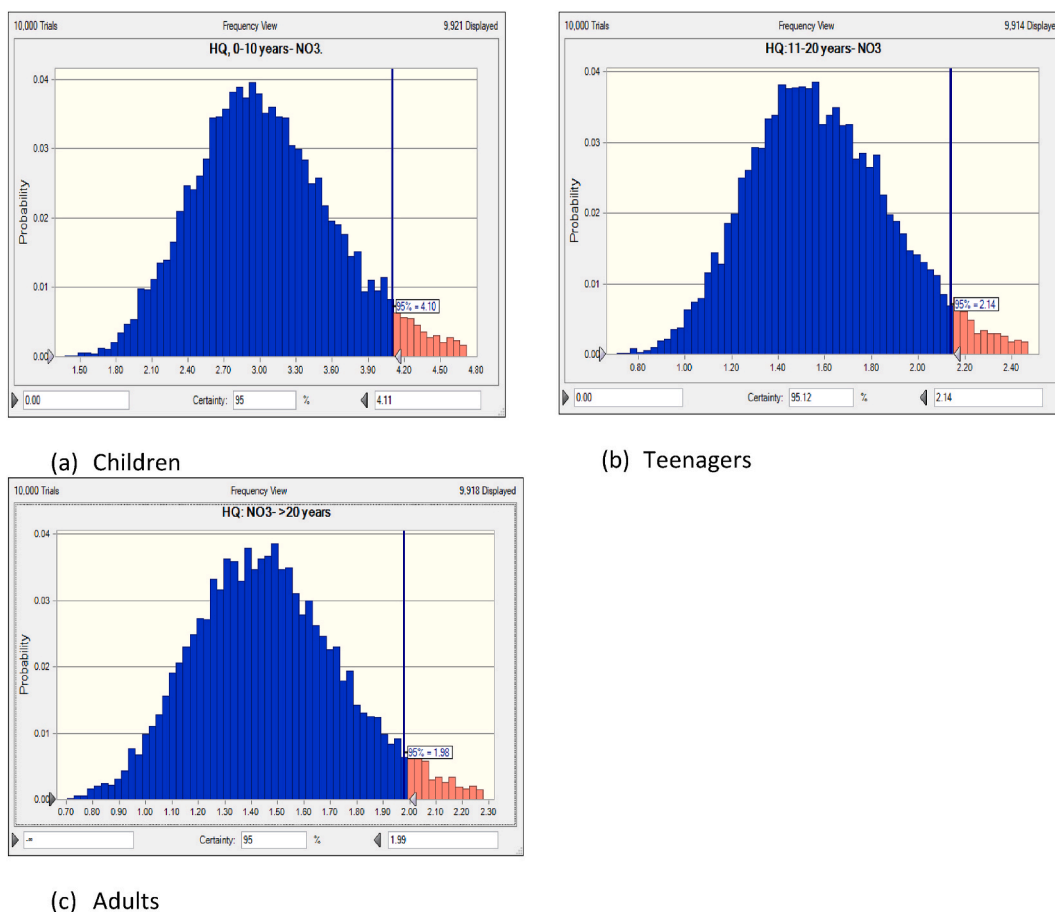


Fig. 7. a, b, c. Bar graphs displaying the results of Nitrate HQ's uncertainty analysis in Children, Teenagers, and Adults groups for the rural Mathura region in U.P, India.

3.2. Assessment of fluoride and nitrate effect on human health

3.2.1. Predestinarianism method

This is a powerful tool that was used to consider the factors involved in the risk measurement of human health and to find the solutions involved in controlling those factors [51]. This tool helps identify the consequences of fluoride and nitrate on the human health of the targeted area. The effect of contaminants on all targeted age groups—children, teenagers, and adults—was calculated using Equation (2), with the results presented in Tables 5 and 6. The spatial distribution and dispersion of fluoride and nitrate among these groups were illustrated by the inverse distance weighting method, as shown in Figs. 4 and 5.

Oral exposure to fluoride and nitrate was evaluated using hazard quotients (HQ) expressed as mg/day and mg/kg/day, respectively. In the proposed work, HQ for all the groups was calculated for the different areas of rural areas of Mathura region, U. P, India and it was found that there is a big difference in the exposure dose of different aged group people of rural areas. In the case of HQ Fluoride in children (0.33–2.67), teenagers (0.17–1.39), and adults (0.16–1.29) and HQ Nitrate in Children (0.02–10.75), teenagers (0.01–5.61), and adults (0.01–5.18). Thus, the average HQ of Fluoride and Nitrate for children, teenager and adult were found to be 1.88, 0.98, 0.90 and 3.02, 1.57, 1.45 respectively. Correspondingly, Tables 4 and 5 showed the maximum HQ of the exposure dose of fluoride and nitrate is found in a rural area of Mathura region 2.67 and 10.75 respectively. The range, however, exceeded the daily limits for F^- and NO_3^- that were determined to be “safe and acceptable” according to the National Radiological Compensation Commission (2001) and USEPA recommendations [17,54,55]. According to the USEPA instructions, $HQ \geq 1$ is not advisable as it leads to severe non-carcinogenic disease in the body.

3.2.2. Probability calculation using the MCS technique

The MCS method was used to determine HQ using equation (2). F^- and NO_3^- concentration, BW, EF, IR, and other data were included in the MCS technique's probabilistic method for all target groups. The mathematical results are shown in Figs. 6 and 7 (a), (b), (c) for all targeted groups exposed.

When HQ values are higher than 1, it means that there is a higher chance of long-term non-cancer and cancer, organ damage in

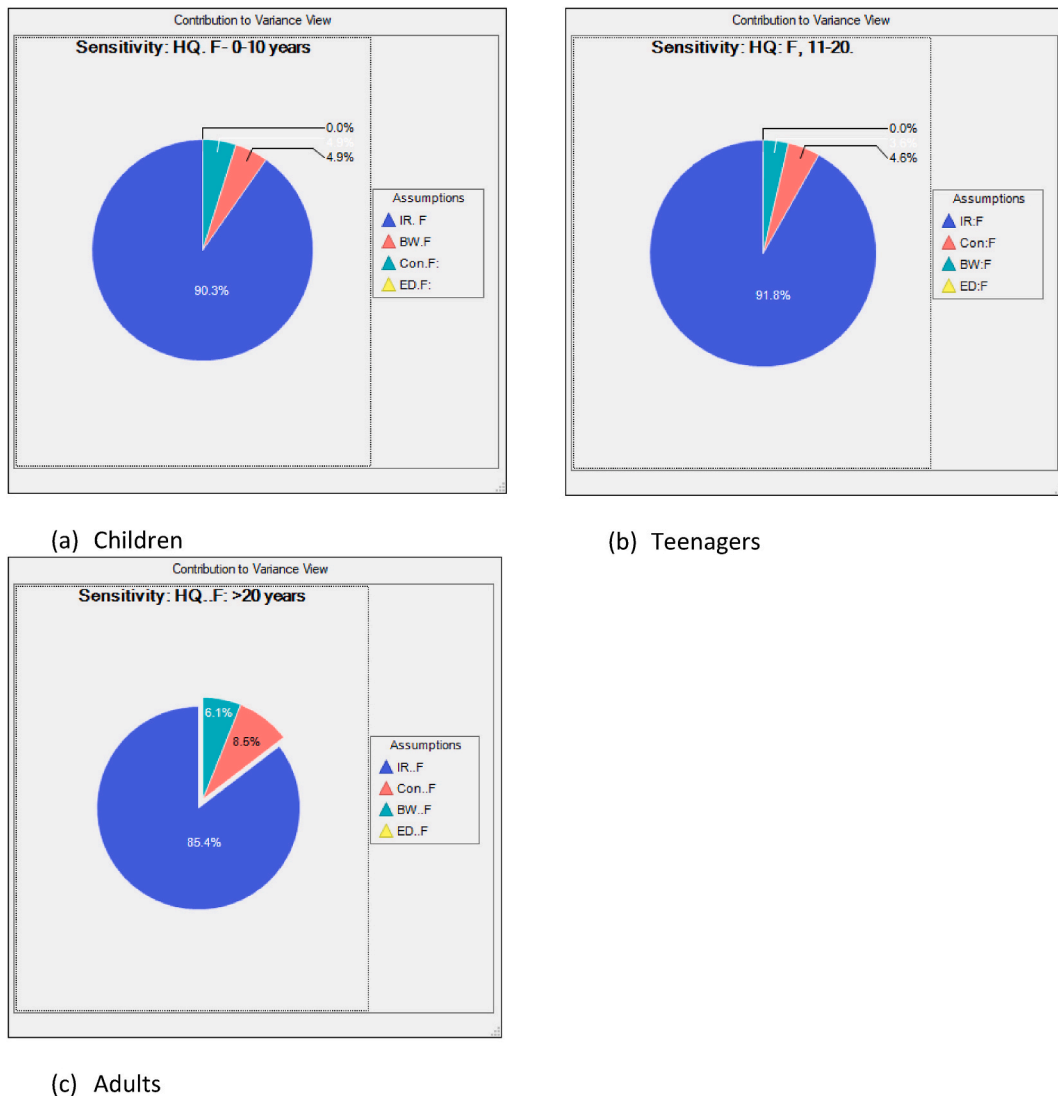


Fig. 8. a, b, c. Fluoride exposure sensitivity investigation Children, Teenagers and Adults rural Mathura, U.P, India.

those who are affected by the exposure. As shown in Figs. 6 and 7 (a, b, c) the rural area of the Mathura region had HQ values (fluoride and nitrate) of 2.87, 1.27, 1.03, and 4.10, 2.14, 1.98 for the age groups of children, teenagers, and adults, respectively. The 95th percentile of HQ values for children are 2.87 and 4.10, at the higher end, signifying high health issues. Similar results were found in the Poldasht city, Northwest of Iran [28], Agra, Uttar Pradesh, India [39], Sanandaj, Kurdistan County[53][53], Iran [49] and north China [40].

HRA consists of two major components: unpredictability and sensitivity, which are independent of each other and cannot be ignored. Lack of accurate information about the various parameters being considered invariably leads to unpredictability. The MCS technique is used to reduce the effect of unpredictability in health risk assessment. Ambiguity is often seen in risk assessment since the USEPA's suggested values might change depending on a person's unique traits or geographic region. A random selection of values for every parameter is incorporated into simulations to remedy this. To determine the degree of uncertainty, a sensitivity analysis was also carried out, with an emphasis on the different input variables and how they could affect the outcomes.

The proposed work is used to evaluate the possible health hazards by doing a sensitivity analysis on a range of input parameters, including C, IR, ED EF, BW, and AT. The selected parameters were chosen at random to create tornado plots and do (SA) for the various target groups of the children, teens, and adults and found the descending order of $IR > C > BW > EF$ (fluoride) and $C > BW > IR > EF$ (Nitrate) for children, teenagers and adults Figs. 8 and 9 (a, b, c). This model used mathematical assessments of drinking water's non-cancerous and carcinogenic risks (HQ-ing). In the rural Mathura region, the metrics that showed the greatest influence on all targeted groups were IR, C (fluoride), and C, BW (Nitrate). Their respective correlation coefficients ranged from 85.4 % to 90.3 %, 4.6 %–8.5 % (Fluoride) and 45.6 %–48.2 %, 26 %–27.4 % (Nitrate). As the sensitivity analysis shows, the probability distributions of IR, C

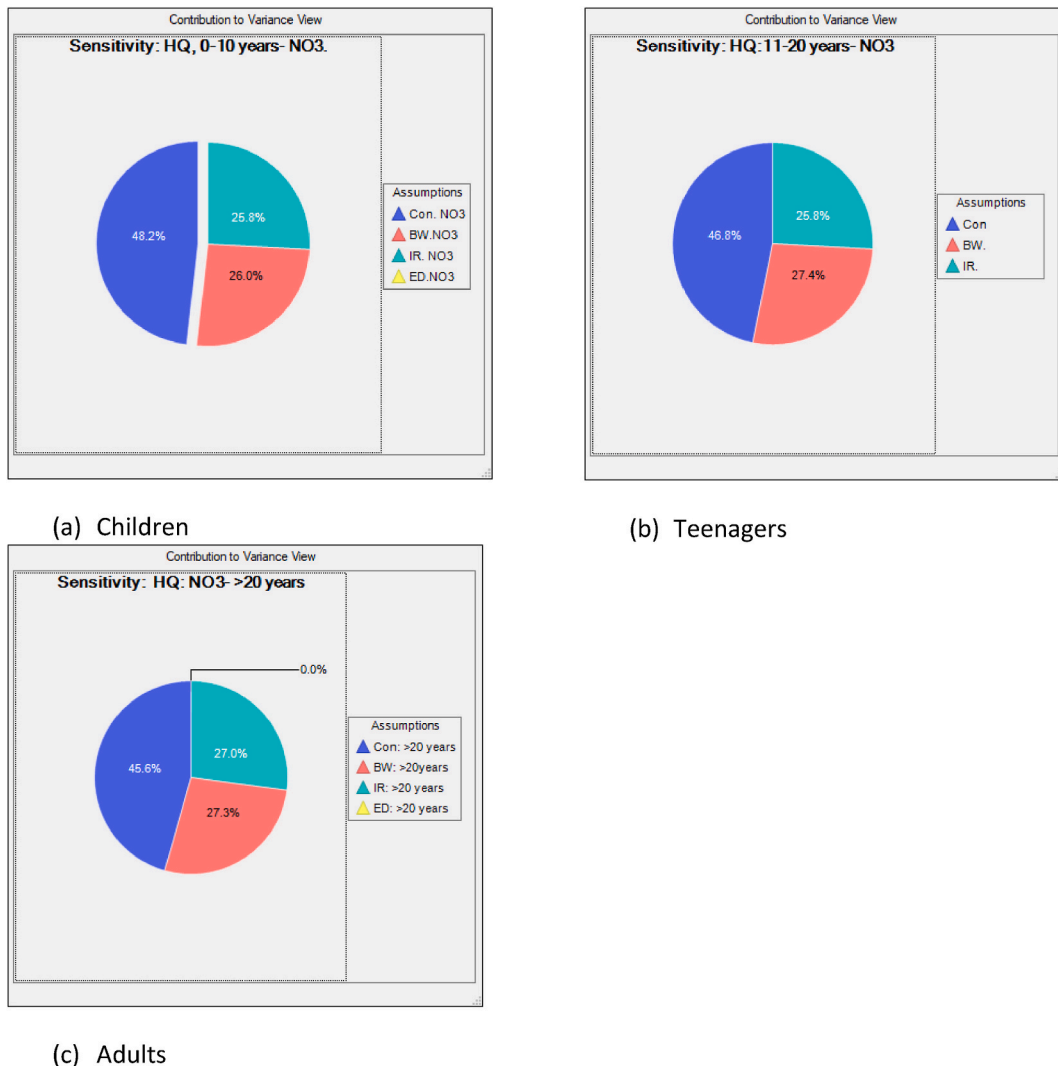


Fig. 9. a, b, c. Nitrate exposure sensitivity investigation Children, Teenagers and Adults groups in rural Mathura, U.P., India.

(Fluoride), and C, BW (Nitrate) turned out to be crucial components in improving the accuracy of the outcomes.

4. Conclusions

In the present study, it was found that the levels of fluoride and nitrate in the groundwater from the rural Mathura region, Uttar Pradesh, India, were far in excess of the recommended limits set by the WHO. A health risk assessment was conducted, which showed a probability of both non-carcinogenic and carcinogenic risks through the consumption of such contaminated groundwater. In particular, HQ values at 95th percentiles for children, teenagers, and adults were higher than the safe zone, thus a major health concern.

The Monte Carlo simulation emphasized high risks for children, which were consistent with high HQ values calculated. Sensitivity analysis revealed that probability distributions of ingestion rate, fluoride concentration, and body weight were key parameters in reducing the uncertainty ranges of risk assessment results. These results indicate that the high levels of fluoride and nitrate are most likely controlled by the peculiar local geological features, which render this groundwater not suitable for human consumption. Considering the severe health risks, treatment of the groundwater of Mathura district has been essentially required to be made safe for drinking purposes. It is also advisable to include alternative sources of potable water as well, so that the health and safety of the community may be safeguarded. The outcome of this study sends clearly a red alert for action to prevent further contamination and adverse health effects from long-term exposure to fluoride and nitrate in the groundwaters and to protect the community.

Data availability statement

Data will be made available on request.

CRediT authorship contribution statement

Shahjad Ali: Writing – original draft, Methodology, Investigation, Conceptualization. **Salman Ahmad:** Writing – original draft, Investigation, Conceptualization. **Mohammad Usama:** Writing – original draft, Methodology, Investigation. **Raisul Islam:** Writing – original draft, Methodology, Investigation. **Azhar Shadab:** Writing – original draft, Software, Investigation. **Rajesh Kumar Deolia:** Writing – original draft, Methodology, Investigation. **Jitendra Kumar:** Writing – original draft, Investigation, Data curation. **Ayooob Rastegar:** Writing – original draft, Software. **Ali Akbar Mohammadi:** Writing – original draft, Methodology, Investigation, Conceptualization. **Shadab Khurshid:** Writing – original draft, Methodology, Investigation. **Vahide Oskoeit:** Writing – original draft, Software, Methodology. **Seyed Alireza Nazari:** Writing – original draft, Investigation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

Authors acknowledge (Sharda University Agra, Keetham Agra-282007 India) for giving the lavatories during the entire research work and also acknowledge (Dr. Salman Ahmad) for supporting to research work.

References

- [1] N. ur Rehman, W. Ali, S. Muhammad, Y. Tepe, Evaluation of drinking and irrigation water quality, and potential risks indices in the Dera Ismail Khan district, Pakistan, *Kuwait J. Sci.* 51 (1) (Jan. 2024) 100150, <https://doi.org/10.1016/j.kjs.2023.11.001>.
- [2] F. Ustaoglu, Y. Tepe, B. Taş, Assessment of stream quality and health risk in a subtropical Turkey river system: a combined approach using statistical analysis and water quality index, *Ecol. Indic.* 113 (Jun. 2020) 105815, <https://doi.org/10.1016/j.ecolind.2019.105815>.
- [3] Y. Tepe, H. Aydin, Water quality assessment of an urban water, batlama creek (Giresun), Turkey by Applying multivariate statistical techniques, *Fresenius Environ. Bull.* 26 (August) (2017) 6413–6420.
- [4] M.A. Khan, et al., Potential health risk assessment, spatio-temporal hydrochemistry and groundwater quality of Yamuna river basin, Northern India, *Chemosphere* 311 (Jan. 2023) 136880, <https://doi.org/10.1016/j.chemosphere.2022.136880>.
- [5] S. Ali, et al., Groundwater quality assessment using water quality index and principal component analysis in the Achnera block, Agra district, Uttar Pradesh, Northern India, *Sci. Rep.* 14 (1) (2024) 1–13, <https://doi.org/10.1038/s41598-024-56056-8>.
- [6] S. Ali, A.A. Mohammadi, H. Ali, N. Alinejad, M. Maroosi, Qualitative assessment of ground water using the water quality index from a part of Western Uttar Pradesh, North India, *Desalination Water Treat.* 252 (2022) 332–338, <https://doi.org/10.5004/dwt.2022.28263>.
- [7] M. Qasemi, et al., Characteristics, water quality index and human health risk from nitrate and fluoride in Kakhk city and its rural areas, Iran, *J. Food Compos. Anal.* 115 (Jan. 2023) 104870, <https://doi.org/10.1016/j.jfca.2022.104870>.
- [8] B. Panneerselvam, K. Muniraj, K. Duraisamy, C. Pande, S. Karuppannan, M. Thomas, An integrated approach to explore the suitability of nitrate-contaminated groundwater for drinking purposes in a semiarid region of India, *Environ. Geochem. Health* 45 (3) (2023) 647–663, <https://doi.org/10.1007/s10653-022-01237-5>.
- [9] M. Golaki, A. Azhdarpoor, A. Mohamadpour, Z. Derakhshan, G.O. Conti, Health risk assessment and spatial distribution of nitrate, nitrite, fluoride, and coliform contaminants in drinking water resources of kazerun, Iran, *Environ. Res.* 203 (Jan. 2022) 111850, <https://doi.org/10.1016/j.envres.2021.111850>.
- [10] M. Ghanbarian, A. Roudbari, S. Nazemi, A.-B. Javid, A comparative study of various parameters of drinking water quality in Shahroud city, Iran: tap water, well water and bottled water, *Water Pol.* 24 (6) (Jun. 2022) 867–877, <https://doi.org/10.2166/wp.2022.201>.
- [11] S. Ali, R.K. Deolia, S. Singh, Physico-chemical characterization of groundwater in terms of water quality index (WQI) for urban areas of Agra, North India 10 (6) (2022) 409–416, <https://doi.org/10.12691/aees-10-6-11>.
- [12] C.R. Ramakrishnaiah, C. Sadashivaiah, G. Ranganna, Assessment of water quality index for the groundwater in tumkur taluk, Karnataka state, India, *E-Journal Chem.* 6 (2) (2009) 523–530, <https://doi.org/10.1155/2009/757424>.
- [13] J. Berman, WHO: Waterborne Disease Is World's Leading Killer, vol. 29, 2009, p. 12.
- [14] A. Malik, A. Yasar, A.B. Tabinda, M. Abubakar, Water-borne diseases, cost of illness and willingness to pay for diseases interventions in rural communities of developing countries, Iran, *J. Public Health* 41 (6) (2012) 39–49.
- [15] S.U. Khan, M. Asif, F. Alam, N.A. Khan, I.H. Farooqi, Optimizing fluoride removal and energy consumption in a batch reactor using electrocoagulation, *A Smart Treatment Technology* (2020) 767–778, https://doi.org/10.1007/978-981-15-2545-2_62.
- [16] Q.S. Mateen, S.U. Khan, D.T. Islam, N.A. Khan, I.H. Farooqi, Copper (II) removal in a column reactor using electrocoagulation: parametric optimization by response surface methodology using central composite design, *Water Environ. Res.* 92 (9) (Sep. 2020) 1350–1362, <https://doi.org/10.1002/wer.1332>.
- [17] S. Ali, H. Ali, M. Pakdel, S. Ghale Askari, A.A. Mohammadi, S. Rezaia, Spatial analysis and probabilistic risk assessment of exposure to fluoride in drinking water using GIS and Monte Carlo simulation, *Environ. Sci. Pollut. Res.* 29 (4) (Jan. 2022) 5881–5890, <https://doi.org/10.1007/s11356-021-16075-8>.
- [18] WHO, Guidelines for drinking-water quality: second addendum, *World Heal. Organ. Press* 1 (2008) 17–19 [Online]. Available: http://www.who.int/water_sanitation_health/dwq/secondaddendum20081119.pdf.
- [19] K.K. Yadav, V. Kumar, N. Gupta, S. Kumar, S. Rezaia, N. Singh, Human health risk assessment: study of a population exposed to fluoride through groundwater of Agra city, India, *Regul. Toxicol. Pharmacol.* 106 (Aug. 2019) 68–80, <https://doi.org/10.1016/j.yrtph.2019.04.013>.
- [20] BIS, Indian standard drinking water specification (second revision), *Bur. Indian Stand. IS 10500* (May) (2012) 1–11 [Online]. Available: <http://cgwb.gov.in/Documents/WQ-standards.pdf>.
- [21] P. Taylor, S. Ayooob, A.K. Gupta, Critical Reviews in Environmental Science and Technology Fluoride in Drinking Water : A Review on the Status and Stress Effects Fluoride in Drinking Water : A Review (August 2013. 2007), <https://doi.org/10.1080/10643380600678112>.
- [22] M.H. Dehghani, A. Zarei, M. Yousefi, F. Baghal Ashgari, G.A. Haghigat, Fluoride contamination in groundwater resources in the southern Iran and its related human health risks, *Desalin. WATER Treat.* 153 (2019) 95–104, <https://doi.org/10.5004/dwt.2019.23993>.

- [23] M. Yousefi, A.A. Mohammadi, M. Yaseri, A.H. Mahvi, Study areas : Poldasht County is located in West Azerbaijan Province in north western Iran with UTM coordinates : zone/sector 39S , 446625 – 513055 m E , and 4344280 – 4402863 m N . The Poldasht meteorological station showed that in the long-term , the, Fluoride 50 (September) (2017) 343–353 [Online]. Available: http://www.fluorideresearch.org/503/files/EJ2017_v50_n3_p343-353_sfs.pdf.
- [24] K.K. Yadav, N. Gupta, V. Kumar, S.A. Khan, A. Kumar, A review of emerging adsorbents and current demand for defluoridation of water: bright future in water sustainability, *Environ. Int.* 111 (Feb. 2018) 80–108, <https://doi.org/10.1016/j.envint.2017.11.014>.
- [25] N. Subba Rao, Controlling factors of fluoride in groundwater in a part of South India, *Arabian J. Geosci.* 10 (23) (Dec. 2017) 524, <https://doi.org/10.1007/s12517-017-3291-7>.
- [26] J. Maurya, S.N. Pradhan, Seema, A.K. Ghosh, Evaluation of ground water quality and health risk assessment due to nitrate and fluoride in the Middle Indo-Gangetic plains of India, *Hum. Ecol. Risk Assess.* 27 (5) (May 2021) 1349–1365, <https://doi.org/10.1080/10807039.2020.1844559>.
- [27] C.P.S. Ahada, S. Suthar, Assessment of human health risk associated with high groundwater fluoride intake in southern districts of Punjab, India, *Expo. Heal.* 11 (4) (Dec. 2019) 267–275, <https://doi.org/10.1007/s12403-017-0268-4>.
- [28] M. Yousefi, M. Ghoochani, A. Hossein Mahvi, Health risk assessment to fluoride in drinking water of rural residents living in the Poldasht city, Northwest of Iran, *Ecotoxicol. Environ. Saf.* 148 (Feb. 2018) 426–430, <https://doi.org/10.1016/j.ecoenv.2017.10.057>.
- [29] R.A. Fallahzadeh, et al., Spatial variation and probabilistic risk assessment of exposure to fluoride in drinking water, *Food Chem. Toxicol.* 113 (Mar. 2018) 314–321, <https://doi.org/10.1016/j.fct.2018.02.001>.
- [30] L. Zhang, et al., Spatial distribution of fluoride in drinking water and health risk assessment of children in typical fluorosis areas in north China, *Chemosphere* 239 (Jan. 2020) 124811, <https://doi.org/10.1016/j.chemosphere.2019.124811>.
- [31] D. Fluoride, N.A. Systematic, A.L. Choi, G. Sun, Y. Zhang, P. Grandjean, *Review* 1362 (10) (2020) 1362–1368.
- [32] S. Ali, M. Kumari, S.K. Gupta, A. Sinha, B.K. Mishra, Investigation and mapping of fluoride-endemic areas and associated health risk—a case study of Agra, Uttar Pradesh, India, *Hum. Ecol. Risk Assess.* 23 (3) (2017) 590–604, <https://doi.org/10.1080/10807039.2016.1255139>.
- [33] S. Ali, S.K. Gupta, A. Sinha, S.U. Khan, H. Ali, Health risk assessment due to fluoride contamination in groundwater of Bichpuri, Agra, India: a case study, *Model. Earth Syst. Environ.* 8 (1) (2022) 299–307, <https://doi.org/10.1007/s40808-021-01105-8>.
- [34] M. Qasemi, et al., Investigation of potential human health risks from fluoride and nitrate via water consumption in Sabzevar, Iran, *Int. J. Environ. Anal. Chem.* 102 (2) (Jan. 2022) 307–318, <https://doi.org/10.1080/03067319.2020.1720668>.
- [35] A. Roudbari, M. Ghanbarian, A.B. Javid, M. Afshari, Investigation of nitrite and nitrate levels in some summer vegetables cultivated in bastam region-shahroud-Iran, *J. Knowl. Heal. Basic Med. Sci.* 17 (3) (2022) 33–39, <https://doi.org/10.22100/jkh.v17i3.2704>.
- [36] A. Temkin, S. Evans, T. Manidis, C. Campbell, O.V. Naidenko, Exposure-based assessment and economic valuation of adverse birth outcomes and cancer risk due to nitrate in United States drinking water, *Environ. Res.* 176 (Sep. 2019) 108442, <https://doi.org/10.1016/j.envres.2019.04.009>.
- [37] A. Azhdarpoor, et al., Assessing fluoride and nitrate contaminants in drinking water resources and their health risk assessment in a Semi-arid region of Southwest Iran, *Desalination Water Treat.* 149 (June) (2019) 43–51, <https://doi.org/10.5004/dwt.2019.23865>.
- [38] A. Mohammadpour, et al., The concentration of cadmium, lead, and nitrate in tomato and onion from Fars province, Iran: a health risk assessment study, *Int. J. Environ. Anal. Chem.* (Dec. 2022) 1–13, <https://doi.org/10.1080/03067319.2022.2151364>.
- [39] S. Ali, et al., Variability of groundwater fluoride and its proportionate risk quantification via Monte Carlo simulation in rural and urban areas of Agra district, India, *Sci. Rep.* 13 (1) (2023) 1–13, <https://doi.org/10.1038/s41598-023-46197-7>.
- [40] L. Huang, Z. Sun, A. Zhou, J. Bi, Y. Liu, Source and enrichment mechanism of fluoride in groundwater of the hotan oasis within the tarim basin, Northwestern China, *Environ. Pollut.* 300 (May 2022) 118962, <https://doi.org/10.1016/j.envpol.2022.118962>.
- [41] S. Ahmed, S. Khurshid, W. Sultan, M.B. Shadab, Statistical analysis and water quality index development using GIS of mathura city, Uttar Pradesh, India, *Desalination Water Treat.* 177 (March) (2020) 152–166, <https://doi.org/10.5004/dwt.2020.24946>.
- [42] S. Ali, H. Ali, M. Pakdel, S. Ghale Askari, A.A. Mohammadi, S. Rezaei, Spatial analysis and probabilistic risk assessment of exposure to fluoride in drinking water using GIS and Monte Carlo simulation, *Environ. Sci. Pollut. Res.* 29 (4) (2022) 5881–5890, <https://doi.org/10.1007/s11356-021-16075-8>.
- [43] L.S. Clesceri, A.E. Greenberg, R.R. Trussell, *Standard Methods for the Examination of Water and Wastewater*, American Public Health Association, Washington DC, 1990.
- [44] EPA, *Risk assessment guidance for superfund, Human Health Evaluation Manual (Part A) I (December) (1989) 289.*
- [45] J. Bazeli, et al., Health risk assessment techniques to evaluate non-carcinogenic human health risk due to fluoride, nitrite and nitrate using Monte Carlo simulation and sensitivity analysis in Groundwater of Khaf County, Iran, *Int. J. Environ. Anal. Chem.* 102 (8) (Jun. 2022) 1793–1813, <https://doi.org/10.1080/03067319.2020.1743280>.
- [46] R.L. Smith, Use of Monte Carlo simulation for human exposure assessment at a superfund site, *Risk Anal.* 14 (4) (1994) 433–439, <https://doi.org/10.1111/j.1539-6924.1994.tb00261.x>.
- [47] S. Ali, et al., Health risk assessment due to fluoride exposure from groundwater in rural areas of Agra, India: Monte Carlo simulation, *Int. J. Environ. Sci. Technol.* 18 (11) (Nov. 2021) 3665–3676, <https://doi.org/10.1007/s13762-020-03084-2>.
- [48] J. Bazeli, et al., Health risk assessment techniques to evaluate non-carcinogenic human health risk due to fluoride , nitrite and nitrate using Monte Carlo simulation and sensitivity analysis in Groundwater of Khaf County , Iran, *Int. J. Environ. Anal. Chem.* 00 (00) (2020) 1–21, <https://doi.org/10.1080/03067319.2020.1743280>.
- [49] C. : :) 11-il-! i-, E. P. A. H. J, 2002, pp. 1–25.
- [50] H. Soleimani, et al., Probabilistic and deterministic approaches to estimation of non-carcinogenic human health risk due to heavy metals in groundwater resources of torbat heydariyeh, southeastern of Iran, *Int. J. Environ. Anal. Chem.* 102 (11) (Sep. 2022) 2536–2550, <https://doi.org/10.1080/03067319.2020.1757086>.
- [51] H. Soleimani, et al., Groundwater quality evaluation and risk assessment of nitrate using Monte Carlo simulation and sensitivity analysis in rural areas of Divandarreh County, Kurdistan province, Iran, *Int. J. Environ. Anal. Chem.* 102 (10) (Aug. 2022) 2213–2231, <https://doi.org/10.1080/03067319.2020.1751147>.
- [52] S. Jones, B.A. Burt, P.E. Petersen, M.A. Lennon, *The effective use of fluorides in public health* 20289 (4) (2005).
- [53] H. Rezaei, et al., Human and ecological risk assessment : an international health-risk assessment related to the fluoride , nitrate , and nitrite in the drinking water in the Sanandaj , kurdistan county , Iran, *Hum. Ecol. Risk Assess.* 0 (0) (2018) 1–9, <https://doi.org/10.1080/10807039.2018.1463510>.
- [54] R.J. Carton, A. Park, *Review of the 2006 United States national research council report 39 (September) (2006) 163–172.*
- [55] M. Radfarad, A. Badeenezhad, A. Mohammadi, M. Yousefi, Desalination and Water Treatment Health risk assessment to fluoride and nitrate in drinking water of rural residents living in the Bardaskan city , arid region, southeastern Iran Health risk assessment to fluoride and nitrate in drinking water of rural r (2019), <https://doi.org/10.5004/dwt.2019.23651>.