### **ORIGINAL PAPER**



# Trace elements human health risk assessment by Monte Carlo probabilistic method in drinking water of Shiraz, Iran

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### Abstract

Risk assessment analysis related to groundwater contamination by heavy metals was performed in the Shiraz city (Iran). We compared the traditional deterministic methodologies with a probabilistic approach based on the concentration of different heavy metals determined from many sampling points. The relationships between the variables by the multivariate statistical analysis were assessed, and the target hazard quotient (THQ) was calculated in children, women, and men groups. Results showed that analyzed water samples were suitable for drinking, although alkaline. Concentrations of the heavy metals were: Zn > Ni > Cu > Se > Co > Sb. The THQ values for non-carcinogenic elements showed no significant risk for population of studied age groups, although a higher THQ value was observed for the water from the northwest and some central areas of city. Mean values of cancer risk for Ni were  $1.77 \times 10^{-5}$ ,  $4.36 \times 10^{-5}$ , and  $3.32 \times 10^{-5}$  in children, women, and men, respectively. The multivariate approach indicated that the carcinogenic risk certainty level was 97.6, 91.2, and 94.3% for children, women, and men, respectively, and the model sensitivity analysis showed that the most effective parameter for carcinogenicity was Ni concentration. The probabilistic analysis also showed the relative influence of geogenic and anthropogenic processes on the quality of the water of Shiraz city. We concluded that risk assessment using a probabilistic approach could be better predictive of chronic exposure to hazardous elements in drinking water, which possibility the implementation of better protective measures than the current deterministic approaches.

Keywords Drinking water · Probabilistic risk assessment · Heavy metals · Monte Carlo simulation · Multivariate analysis

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# Introduction

Freshwater represents less than 3% of all water on our planet, and groundwater availability and quality are vital natural resources for human beings. Actuality, more than 30% of the world's population relies on groundwater for drinking

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water, especially in arid and semi-arid regions (Jamshidi et al. 2021). Continuous urbanization, industrialization, poor management of waste and industrial effluents, and agricultural activities represent major threats to groundwater quality due to the release of persistent pollutants such as potentially toxic elements (PTEs) (Soleimani et al. 2020b).

Some PTEs, such as Zn, Ni, Cu, Se, Co, are essential in low concentrations for healthy development of human well-being, and living organisms' function (Organization 1996). Some others, e.g., As, Cd, Pb, Sb, are not required for biological functions and are toxic even at low concentrations (Sharafi et al. 2019; Soleimani et al. 2020a). Kidney damage, degenerative neurological conditions, respiratory and cardiovascular disease, and cancer have been reported through groundwater contamination to PTEs (Badeenezhad et al. 2021). Due to their immutable nature, PTEs are persistent, and their accumulation in groundwater represents a primary route of exposure for humans (Kiani et al. 2022). For these reasons, the concentration of several PTEs is regularly monitored by public Authorities to prevent potential hazards to public health.

Risk assessment is a systematic process aiming at determining human exposure to significant risks and implementing control actions to decrease exposure to acceptable levels (Raza et al. 2017). Risk assessment related to groundwater contamination by PTEs is generally conducted by deterministic approaches considering point estimators (Moghtaderi et al. 2020; Abolfazli et al. 2021). While consensual, this approach to risk assessment, does not take into account natural variability, data uncertainty, measurement uncertainty, and eventual lack of environmental data. The point estimation approach also does not account for the dispersion of the analytical data around mean values, being based on fixed equal weights to all of the available data. whereas Differently, the probabilistic risk assessment approach is a more comprehensive methodology for evaluating risks related to environmental pollution (Gebeyehu and Bayissa 2020; Silvestri et al. 2021), because its statistic representation can encompass all or selected subsets of the physical and chemical environmental features. For example, it considers the actual concentration range of each PTEs in groundwater of a given area in time and space, not only mean values. Hence, the multivariate approach to risk assessment can lead to more proper risk assessment and sustainable risk prevention measures. This approach is based on using all data in a distribution function, which can significantly improve the risk assessment by accounting for the spatial variability and other main factors of the studied environment (Rivera-Velasquez et al. 2013; Shahsavani et al. 2023), especially if coupled with sensitivity analysis.

Iran, like other arid and semi-arid areas, relies 60% on groundwater for freshwater supply, with an increasing trend of use (Karamia et al. 2019), but risk assessment using probabilistic approaches to the water quality in Iran is still scarce. Shiraz, the most important city in Southern Iran, is faced with urban sprawl and vegetation decline, increasing drilling of deeper wells to reach lower groundwater levels, and a significant increase in the pressure on natural resources. Among the probabilistic approaches for risk assessment, the Monte Carlo method is one of the most widely used, especially for large monitoring surveys (Kavcar et al. 2006). In this study, the concentration of some toxic elements in the drinking water of Shiraz city was determined and their spatial distribution was drawn using ArcGIS software. To identify the sources of pollution and the relationships between different parameters, multivariate statistical analysis techniques were used. Finally, the health risk assessment and distribution patterns of different PTEs in groundwater were conducted on the drinking water of the city of Shiraz, South Iran, using both a deterministic and a probabilistic approach based a Monte Carlo simulation. This study illustrates how a probabilistic approach can provide more robust results for land planning and implementing appropriate groundwater preservation measures and actions for better protecting human health in complex urban areas where groundwater presents broad ranges of concentration of different PTEs.

# Materials and methods

#### Study area

The present study was conducted in the city of Shiraz in SW Iran (52°29'E, 52°36 29° 33 ', 29°36' N), the Fars province (Fig. 1). Shiraz city has a population of more than 1.5 million people and covers an area of 240 km<sup>2</sup>, and drinking water wells are scattered in the urban area boundary line (Fig. 1). The geology of the Shiraz area includes Asmari, Razak, and Razzaq formations in the mountainous region of Zagros, forming closed basins of central Iran, characterized by alkaline and sodic soils developed from chalky marl parent rocks. The climate is temperate, with an average annual temperature of 18.6° C, precipitation amounting to 325.6 mm that represents the primary source of water supply in the area, and wind speed of 2.35 m/s (Keshavarzi et al. 2015).





Fig. 1 The geographic position of sampling sites in the distribution network of Shiraz city

### Water sampling and chemical analysis

Fifty-nine samples were taken from Shiraz urban drinking water plumbing and transmission system based on the population distribution in the summer 2021 selected with a spatial distribution developed using Arc GIS 10.3 software (ESRI, Redlands, CA, USA), (Aleem et al. 2018). A global positioning system (GPS) was applied to locate the sampling points, the World Geodetic System (WGS-1984) was used to fix the selected points, and the inverse distance weight (IDW) method was applied to draw the spatial distribution of heavy metal concentration in the study area (Mosaferi et al. 2014).

Polyethylene bottles previously washed with distilled water, and 20% HNO<sub>3</sub> were used to collect water samples. Water samples were filtered using Whatman filters with pores of 0.45  $\mu$ m to prevent adsorption and crystallization of trace elements. Then, 3 ml of 69% HNO<sub>3</sub> was added to each sample to prevent turbidity due growth of microbial colonies prior to elemental analysis and shipped to the analytical laboratory in refrigerated at 4 °C boxes. Concentrations of cobalt (Co), nickel (Ni), copper (Cu), zinc (Zn), selenium (Se), and antimony (Sb) were measured by Inductively

Coupled Plasma followed by Mass Spectrometry (ICP-MS Agilent 7800, USA). Total dissolved solids (TDS), electrical conductivity (EC), and pH values of all samples were measured by a conductivity meter (WTW Cond 720) and pH meter (Metrom, Model 827), respectively. All determinations were performed in triplicates.

### Health risk assessment

#### **Deterministic approach**

Because in most studies, the amount of carcinogenic risk in the adult group and the non-carcinogenic risk in the children group is higher than the other age groups, for this reason the city population was divided into three age groups: children (<6 years), adult women (20–70 y), and adult men (20–70 y), age groups generally accepted in environmental risk assessment (Mohammadi et al. 2017). The Chronic Daily Intake, i.e., the average daily dose (CDI) for the analyzed elements, was calculated according to (Joodavi et al. 2021; Shafiuddin Ahmed et al. 2021) using the following equation:



$$CDI = \frac{C \times IR \times EF \times ED}{BW \times AT}$$
(1)

where Ci is the average contamination concentration in water (mg l<sup>-1</sup>), IR is the ingestion rate of water (l d<sup>-1</sup>, EF is the exposure frequency (d year<sup>-1</sup>), ED is the exposure duration for cancer risk assessment (years), BW is the average body weight (kg), AT is the averaging time (day). According to the USEPA, the threshold values for the carcinogenic risks posed by the analyzed elements were in the range of  $10^{-6}$ – $10^{-4}$ , unacceptable for CDI >  $10^{-4}$  (Ogamba et al. 2021). The following equation calculated the carcinogenic risk for Ni:

$$CR = \Sigma CDI \times SF \tag{2}$$

where CDI is the Chronic Daily Intake and S.F. is the cancer slope factor, which differs for each element (Farokhneshat et al. 2016). The following equation calculated the target hazard quotient (THQ):

$$THQ = \sum \frac{CDI_i}{RfD_i}$$
(3)

where the RfD is the Reference Dose value of each element based on the (US EPA 1989) screening level values (EPA 1989).

### **Probabilistic approach**

The PTEs analytical data were modeled with a probabilistic approach to improve the risk assessment by the Monte Carlo method coupled with a sensitivity analysis (Soleimani et al. 2020a). Input values for Monte Carlo simulation and sensitivity analysis are reported in Table 1.

The Crystal Ball®software, an 'add-in for Microsoft Excel, was used to perform analysis, produce the input distribution values, collect the output graphically, and calculate summary statistics, and the distribution factor of heavy metals concentration can be obtained in the 'Definition assumption' tool of the Crystal Ball® software (Shalyari et al. 2019). Because no distribution parameters were available from previous studies conducted in the area, the other probability distribution functions employed in the sensitivity analysis (SA) and Monte Carlo simulation were those suggested by the U.S. Environmental Protection Agency (Fitzpatrick et al. 2017).

Table 1 Parameters used in Monte Carlo Simulation and uncertainty analysis

Symbol	Parameter	Unit	Distribution Factor	Value	References
С	Contaminant concentration	mg l <sup>-1</sup>	_		_
IR	Ingestion rate	$1  day^{-1}$	Log-normal	Children = [1.25, 0.57]	Fallahzadeh et al. (2018), Wang
				Women = [2.22, 0.57]	et al. (2020), Bazeli et al. (2020)
				Men = [2.37, 0.85]	
EF	Exposure frequency	days year <sup>-1</sup>	Triangular	Children = [180, 345,365]	
				Women = [[180, 345, 365]	
				men=[180, 345,365]	
ED	Exposure duration	Year	Fixed	Children=6	
				Women=50	
				Men = 50	
BW	Body weight	Kg	Log-normal	Children = [10.64, 3.79]	
				Women=[57.03, 1.10]	
				Men=[78, 3.9]	
AT	Averaging lifetime	Days	Fixed	Non-carcinogenic = $ED \times 365$ carcinogenic = $70 \times 365$	
SF	Slope factor	mg <sup>-1</sup> kg day	Fixed	Ni=1.7	Fallahzadeh et al. (2017)
RfD	Reference dose	${ m mg}~{ m kg}^{-1}~{ m day}^{-1}$	Fixed	Co=0.02	Bortey-Sam et al. (2015), Wu et al.
				Ni=0.02	(2009)
				Cu=0.04	
				Zn = 0.3	
				Se=0.005	
				Sb = 0.0004	



# Principle component analysis and cluster analysis method

# The use of principal component analysis (PCA) is one of the most common environmetric techniques for determining the contributions of human and natural resources (Nasir et al. 2011). The application of PCA is for comparing the compositional and spatial patterns of water samples and finding possible sources of trace metals in them (Barakat et al. 2016).

Because heavy metals enrichment in groundwater is influenced by site-specific factors such as rock-mineral weathering, drainage density, geological and hydro-geological settings, and anthropogenic activities, we used the Hierarchical Cluster Analysis (HCA) method to classify water samples in quality classes and assess the dissimilarities between different classes. Ward's linkage method, including squared Euclidean and z-score standardization, was used for analysis.

## **Data analysis**

Statistical analysis was performed using IBM SPSS software (version 16; SPSS Inc., Chicago, IL, USA). Nonparametric tests were used to analyze the results since the data were not normally distributed, which was determined by the Kolmogorov–Smirnov test (P < 0.05). Then, the uncertainty analysis was calculated using Oracle Crystal Ball software (version 11.1.2.3). Spatial analysis of geochemical data was performed by inverse distance weighting (IDW) using Arc-GIS software (10.8). PCA and the cluster analysis method used software by IBM SPSS software.

## **Results and discussion**

# PTEs Concentration in drinking water and spatial variation

Mean values and ranges of PTEs concentrations in drinking water samples from Shiraz city are reported in Table 2.

All groundwater samples had a sub-alkaline alkaline pH value (Table 2), with an average pH value of 7.91 due to the presence of soluble carbonates, mainly bicarbonate  $(HCO_3^{-})$  ions (Adams et al. 2001).; This result was expected due to the geological features of the Shiraz area. The average value of water EC was 643  $\mu$ S cm<sup>-1</sup>, with all values below the recommended maximum threshold value for drinking water (Table 2). The range of TDS concentrations had an average value of 257 mg  $1^{-1}$ , all samples had values below the maximum threshold recommended by the US EPA (Table 2), although some samples presented values (e.g., 481 mg  $l^{-1}$ ) to the maximum admissible value. The TDS value of water is an important parameter in determining the water quality for human consumption because high levels of TDS in waters are generally due to Na, K, and chlorides which may affect human health upon prolonged exposure. Waters with high TDS values are also considered unsuitable for irrigation. According to (Rusydi 2018), based on the TDS values the water can be classified into four categories: freshwater (TDS < 1 g  $l^{-1}$ ), brackish waters (1 < TDS < 10 g  $l^{-1}$ ), saline waters ( $10 < TDS < 100 \text{ g l}^{-1}$ ), and brine waters (TDS > 100 g  $l^{-1}$ ). According to this classification, all the analyzed water samples could be considered freshwater.

Mean concentrations and concentration ranges of the measured PTEs are reported in Table 2, and ranked

Contaminant	Concentrations ( $\mu$ g. L <sup>-1</sup> )		Threshold levels ( $\mu$ g l <sup>-1</sup> )	Reference legislation	Threshold levels(µg. L <sup>1</sup> ) ISIRI 1053 WHO		References	
	Min Mean Max							
Со	0.12	0.21	0.46	1	NC DEQ 15A NCAC 02L Groundwater			Tomlinson et al. (2019)
Ni	0.18	1.36	21.32	100	Quality Standard	70		
Zn	0.06	9.62	122.29	1300		-	3	
Cu	0.00	0.56	4.47	2000	U.S. EPA Treatment Technique Action Level	-		
Se	0.06	0.23	0.44	50	U.S. EPA Maximum Contaminant Level	10		
Sb	0.02	0.09	1.02	6		20		
pН	7.68	7.91	8.16	6.5-8.5	WHO	6.5-8.5		
TDS (mg $l^{-1}$ )	128	257	481	500		1500		Karunanidhi et al. (2021)
$EC~(\mu S~cm^{-1})$	321	643	1203	1500		-		

Table 2 Descriptive statistics of physicochemical properties and elemental concentrations in the water samples of Shiraz city



as it follows:6 Zn (9.62) > Ni (1.36) > Cu (0.56) > Se (0.23) > Co (0.21) > Sb (0.09). Means concentrations and concentration ranges for the studied PTEs in the ground-water of Shiraz city were comparable to those reported by Tavanpour et al. (2016), who attributed the relatively high Zn concentrations in water samples to their natural occurrence or the corrosion of galvanized pipes; however, though all mean values of PTEs concentrations were below the recommended threshold limits, the broad concentration ranges observed for several PTEs clarify the need for a probabilistic approach for a more reliable risk assessment.

Spatial distribution maps of the studied trace elements observed using the IDW method in GIS software showed that high Sb, Ni, and Co concentrations were mainly located in the northwest of the city area, whereas waters of the central part of the city were characterized by higher concentrations of Cu, Zn, and Co (Fig. 2). Enrichment with Ni in the waters of the northwest of the city could be attributed to the advanced corrosion of metal pipes and pipe fittings in contact with drinking water (Adhikari et al. 2021). In contrast, galvanic reactions at the boundary between copper pipes and brass fittings in the household plumbing system could be responsible for higher Cu concentrations of water in the city central area (Harvey et al. 2016). Concerning Ni contamination in suburban areas, groundwater contamination in agricultural soils, could be attributed to the use of wastewater for irrigation.

### Multivariate analysis of elements in drinking water

Cluster analysis of water quality parameters showed four distinct clusters, one formed by TDS and EC values and Cu and Zn concentrations, and a second cluster formed by Ni, Sb, and Co concentrations, whereas Se concentration and pH value clustered separately (Fig. 3). While sub-clustering of TDS and EC values could be expected because suspended soils generally exhibit sorption sites for alkaline metals on their surface, clustering of EC and TDS with Cu and Zn concentrations could indicate a potential association of these PTEs with dissolved solids, which in turn could have adverse effects on human health. Possible sources of Pb and Zn can be leachates and/or leakage from hazardous waste dumpsites or uncontrolled release into industrial effluents. Cluster of Ni, Sb, and Co elements may have originated from geogenic sources or anthropogenic activities such as improper waste management, use of phosphate fertilizers and fossil fuels in agriculture, release of wastewater from chemical industry (Moghtaderi et al. 2020).

The PCA Factor loading for the first three principal components with maximum variance, accounting for 71.7% of the total variance, is shown in (Table 3). The PC1 accounted for 28.2% of the total variance and included the TDS and EC (positive loading) and pH (negative loading), the PC2 accounted for 23.6% of the total variance and included Sb, Ni and Co concentrations, whereas the third PC3 accounted for 19.9% of the total variance and included Cu and Zn concentrations (Table 3). The PC1 showed that the interaction between rock substrate and water increases the concentration of dissolved ions in groundwater, and the negative relationship with pH is related to the carbonate origin. Human activities, especially industry, agriculture, untreated sewage, and landfill leachate, could be possible sources of PTEs loaded in PC2, whereas Copper and Zn loaded in PC3 could be attributed to the use of fertilizers, and accumulation of pesticides or fungicides in agricultural soils, acting as secondary source toward groundwater (Qishlaqi and Moore 2007).

The positive coefficients for all of the measured parameters loaded on PC1 and PC2, except for the pH value, indicated that the measured parameters were related among them, and that all of them are influenced by the pH value of the studied waters (Fig. 4).

### Health risk assessment

The minimum, mean and maximum values of the CDI and THQ for different population age groups in the study area are reported in Tables 4 and 5.

The THQ index value obtained for each age group was generally < 1; however, higher THQ values were observed for the population living in the northwest of the urban areas and small city center areas (Table 5).

Mean CR values calculated on the base of the Ni concentration were  $2.19 \times 10^{-5}$  for children,  $6.06 \times 10^{-5}$  for women, and  $4.73 \times 10^{-5}$  for men, indicating moderate carcinogenic risk for all three population age groups, whereas the CR values ranged between  $10^{-6}$  and  $10^{-4}$  for all of the population groups (Table 6).

The spatial variation map of THQ and CR in children and women showed that carcinogenic risks due to Ni intake through the consumption of drinking water in higher in the northwest of the city area (Fig. 5a, b). Appropriate monitoring and protective measures should be taken to reduce the risk in that area of Shiraz city.

In a survey on the quality of the drinking water of Shiraz city, Abolfazli et al. (2021) reported Hazard Quotient (HQ) values < 1 for different PTEs, but a carcinogenic risk for Cr 30 times higher than the permissible limit, with higher cancer and non-cancer risks for children than adults. Sener et al. (2016) reported that HQ values for Cu, Ni, and Zn children were equal to  $(1.21^{-2}-9.09^{-3})$ ,  $(1.07^{-2}-3.35^{-4})$ , and  $(1.68^{-2}-9.96^{-4})$  and in the adult, the group was equal to  $(1.29^{-2}-9.97^{-3})$ ,  $(1.02^{-3}-1.45^{-4})$  and  $(1.14^{-3}-9.15^{-5})$ , indicating low HQ values for the studies area. Values of CDI of Cu



Fig. 2 Spatial distribution maps of Co a, Ni, b Cu, c Zn, d Se, e and Sb, f concentrations in waters samples of Shiraz city





Fig. 3 Cluster analysis of elements and physicochemical properties of the water samples

Table 3 Principal component analysis of elements in drinking water

	Component matrix <sup>a</sup> Component							
	Factor1	Factor2	Factor3					
TDS	0.844	0.027	0.383					
EC	0.845	0.025	0.382					
pH	-0.736	-0.047	0.056					
Co	0.500	0.545	0.021					
Ni	-0.004	0.906	0.334					
Cu	0.261	0.017	0.663					
Zn	0.183	0.318	0.819					
Se	0.463	0.132	-0.515					
Sb	0.007	0.941	-0.078					
Eigenvalue	2.536	2.125	1.790					
Total variance (%)	28.174	23.611	19.891					
Cumulative variance (%)	28.174	51.785	71.676					

Rotation Method: Varimax with Kaiser Normalization

Component Plot in Rotated Space 1.0 0.5 Component 2 pH 0.0 FC -0.5 -1.0 0.5 0.0 -0.5 1.0.0 -1.0 **Component 1** 

Fig. 4 PCA biplot indicates the rotational space changes and the direction and length of the vectors of each variable in the first two principal components

in the tap water of the Kerman region for children and adults of  $3.9 \times 10^{-5}$  and  $1.74 \times 10^{-5}$  mg kg<sup>-1</sup> d<sup>-1</sup>, respectively, were by (Abedi Sarvestani and Aghasi 2019).

Estimation of the probability of developing adverse effects on the health of children, women, and men related to exposure time and concentration of the studied PTEs by the calculation of THQ<sub>95%</sub> values by the Monte Carlo simulation of non-carcinogenic risk resulted in values of 0.09 for the children and 0.02 for the men and women groups therefore below the threshold of 1 (Fig. 6).

Estimation of carcinogenic risk for Ni indicated higher CR values in the following ranking order: women > men > children (Fig. 7). Simulation results showed that the  $CR_{95\%}$  values in the population groups were  $1.47 \times 10^{-4}$  for women,  $1.10 \times 10^{-4}$  for men, and  $6.24 \times 10^{-5}$ for children, indicating carcinogenic risk in all population groups (Fig. 7). Higher carcinogenic risk in men and women could be related to their longer exposure duration (ED) than children, but also the higher water intake-to-body weight

Table 5	Total Hazard Quotient
values for	or the measured trace
element	s for the different
populati	on groups

	THQ values									
	Children			Women			Men			
	Min	Mean	Max	Min	Mean	max	min	Mean	Max	
Co	0.0007	0.0012	0.0026	0.0002	0.0004	0.0008	0.0002	0.0003	0.0007	
Ni	0.0010	0.0075	0.1184	0.0003	0.0025	0.0392	0.0003	0.0019	0.0306	
Cu	0.0000	0.0016	0.0124	0.0000	0.0005	0.0041	0.0000	0.0004	0.0032	
Zn	0.0000	0.0036	0.0453	0.0000	0.0012	0.0150	0.0000	0.0009	0.0117	
Se	0.0012	0.0050	0.0099	0.0004	0.0017	0.0033	0.0003	0.0013	0.0026	
Sb	0.0046	0.0243	0.2823	0.0015	0.0080	0.0935	0.0012	0.0063	0.0730	
THQ	0.0177	0.0431	0.4176	0.0059	0.0143	0.1384	0.0046	0.0111	0.1080	



CDI										
Children			Women			Men				
Min	Mean	Max	min	Mean	Max	min	Mean	Max		
$1.32 \times 10^{-5}$	$2.34 \times 10^{-5}$	$5.13 \times 10^{-5}$	$4.38 \times 10^{-6}$	$7.75 \times 10^{-6}$	$1.70 \times 10^{-5}$	$3.42 \times 10^{-6}$	$6.05 \times 10^{-6}$	$1.33 \times 10^{-5}$		
$2.00 \times 10^{-5}$	$1.51 \times 10^{-4}$	$2.37 \times 10^{-3}$	$6.62 \times 10^{-6}$	$4.99 \times 10^{-5}$	$7.84 \times 10^{-4}$	$5.17 \times 10^{-6}$	$3.89 \times 10^{-5}$	$6.12 \times 10^{-4}$		
NC	$6.26 \times 10^{-5}$	$4.96 \times 10^{-4}$	NC	$2.07 \times 10^{-5}$	$1.64 \times 10^{-4}$	NC	$1.62 \times 10^{-5}$	$1.28 \times 10^{-4}$		
$6.48 \times 10^{-6}$	$1.07 \times 10^{-3}$	$1.36 \times 10^{-2}$	$2.15 \times 10^{-6}$	$3.54 \times 10^{-4}$	$4.50 \times 10^{-3}$	$1.68 \times 10^{-6}$	$2.76 \times 10^{-4}$	$3.51 \times 10^{-3}$		
$6.17 \times 10^{-6}$	$2.50\times10^{-5}$	$4.94 \times 10^{-5}$	$2.04 \times 10^{-6}$	$8.28 \times 10^{-6}$	$1.64\times10^{-5}$	$1.60 \times 10^{-6}$	$6.46 \times 10^{-6}$	$1.28\times10^{-5}$		
$1.85\times10^{-6}$	$9.71 \times 10^{-6}$	$1.13 \times 10^{-4}$	$6.13 \times 10^{-7}$	$3.22 \times 10^{-6}$	$3.74 \times 10^{-5}$	$4.79 \times 10^{-7}$	$2.51 \times 10^{-6}$	$2.92\times10^{-5}$		
	$\begin{tabular}{ c c c c } \hline CD1 \\ \hline Children \\ \hline Min \\ \hline 1.32 \times 10^{-5} \\ 2.00 \times 10^{-5} \\ NC \\ 6.48 \times 10^{-6} \\ 6.17 \times 10^{-6} \\ 1.85 \times 10^{-6} \\ \hline 1.85 \times 10^{-6} \end{tabular}$	CDI           Children           Min         Mean $1.32 \times 10^{-5}$ $2.34 \times 10^{-5}$ $2.00 \times 10^{-5}$ $1.51 \times 10^{-4}$ NC $6.26 \times 10^{-5}$ $6.48 \times 10^{-6}$ $1.07 \times 10^{-3}$ $6.17 \times 10^{-6}$ $2.50 \times 10^{-5}$ $1.85 \times 10^{-6}$ $9.71 \times 10^{-6}$	CDI           Children           Min         Mean         Max $1.32 \times 10^{-5}$ $2.34 \times 10^{-5}$ $5.13 \times 10^{-5}$ $2.00 \times 10^{-5}$ $1.51 \times 10^{-4}$ $2.37 \times 10^{-3}$ NC $6.26 \times 10^{-5}$ $4.96 \times 10^{-4}$ $6.48 \times 10^{-6}$ $1.07 \times 10^{-3}$ $1.36 \times 10^{-2}$ $6.17 \times 10^{-6}$ $2.50 \times 10^{-5}$ $4.94 \times 10^{-5}$ $1.85 \times 10^{-6}$ $9.71 \times 10^{-6}$ $1.13 \times 10^{-4}$	$\begin{tabular}{ c c c c c c } \hline CDI & & & & & & & & & & & & & & & & & & &$	$\begin{tabular}{ c c c c c c } \hline CDI & & & & & & & & & & & & & & & & & & &$	$\begin{tabular}{ c c c c c c } \hline CDI & & & & & & & & & & & & & & & & & & &$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		

NC Not calculated

Table 6         Cancer risk (CR)           level for Ni calculated for the		CR									
different population groups.		Children			Women			Men			
values in bold indicate unacceptable risk		Min	Mean	Max	Min	Mean	Max	Min	Mean	Max	
	CR	2.91.10-6	2.19.10-5	3.45.10-4	8.04.10-6	6.06.10-5	9.52 <sup>.</sup> 10 <sup>-4</sup>	6.28 <sup>.</sup> 10 <sup>-6</sup>	4.73 <sup>.</sup> 10 <sup>-5</sup>	7.43.10-4	



Fig. 5 Spatial distribution map of CR and THQ in a women b children groups from drinking water

ratio ( $\frac{IR}{BW}$ (men) <  $\frac{IR}{BW}$ (women) which is higher in women compared to men.

The sensitivity analysis to assess the main factors influencing carcinogenic and non-carcinogenic risks in the three population groups showed that the ingestion rate (IR) and Sb concentration for women were the main variables affecting the non-carcinogenic risk (Figs. 6, 7). In contrast, Ni concentration was the most critical factor for the carcinogenic risk for all three population groups.



Fig. 6 Trends of the non-carcinogenic risk and sensitivity analysis for the groups of children a women, b and men c obtained by Monte Carlo simulation



Fig. 7 Carcinogenic risk and sensitivity analysis of Ni for a Children, b Women, c Men group



The presented results can complement other population exposure data, such as that of airborne  $PM_{10}$  associated with traffic emissions, which have been recently found to exceed the US EPA levels in the Shiraz urban area, and it cannot be excluded that deposition and leaching of airborne particulate matter could contribute to groundwater enrichment with Zn and other trace elements in the critical city center area. Such anthropogenic factors have been proven to be additional sources of PTEs of groundwater to the natural sources (Soleimani et al. 2022; Sharafi et al. 2022).

# Conclusion

The present study showed that different concentrations of various trace elements in drinking water cause different exposure levels to non-carcinogenic and carcinogenic risks for different age and gender groups living in the Shiraz urban area. Risk assessment evidenced risks due to Zn, Ni, Cu, Se, Co, and Sb in groundwater, which was below the acceptability threshold of 1. The model simulation confirmed that the carcinogenic risk assessment results were below the  $1 \times 10-4$ , highlighting Sb concentration as the most impacting element in carcinogenic risk for children, men, and women. Our work showed that risk assessment of the probabilistic approach better predicted human exposure to different PTEs and in different city areas compared to the deterministic one and highlighted the factors that influence the obtained results by the sensitivity analysis. Though Ni concentration in water resulted lower than the legislation limits, monitoring the transmission lines, especially in the northwest of the city, should not be relaxed. This approach could be taken into account by the land-use and land planning Authorities, for example in the sight of the city development towards the northwest are, where groundwater quality may be lower than in other city areas, or where new industrial and commercial sites may further impact the water resources.

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### Declarations

**Conflict of interest** All the authors declare that they have no conflict of interest.

Ethics approval and consent to participate Not applicable.

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