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Occurrence of BTX and PAHs in underground drinking water of coking contaminated sites: Linkage with altitude and health risk assessment by boiling-modified models

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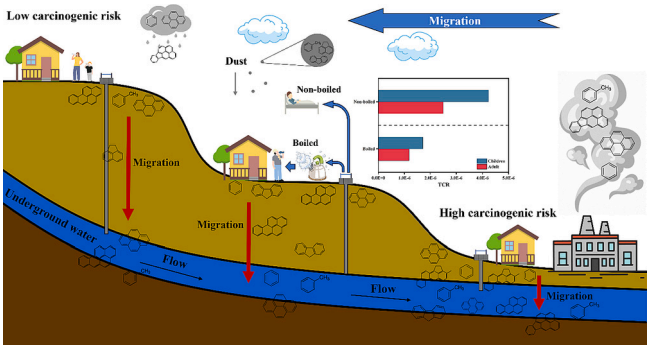
HIGHLIGHTS

- PhMe, BEN, ACE, FLU and PYR dominated in groundwater of coking contaminated sites.
- Concentrations of BTX and PAHs were negatively correlated with altitude.
- Source of BTX/PAHs in residential area originated from coking industrial activities.
- Residual ratios after boiling were determined and used to modify risk assessment model.
- Boiling was an effective strategy to reduce the carcinogenic risks from BTX/PAHs.

GRAPHICAL ABSTRACT



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ABSTRACT

The safety of underground drinking water has received widespread attention. However, few studies have focused on the occurrence and health risks of pollutants in underground drinking water of coking contaminated sites. In this study, the distribution characteristics, sources, and human health risks of benzene, toluene, xylene (BTX) and polycyclic aromatic hydrocarbons (PAHs) in underground drinking water from a typical coking contaminated site in Shanxi of China were investigated. The average concentrations of BTX and PAHs in coking plant (CP) were 5.1 and 4.8 times higher than those in residential area (RA), respectively. Toluene and Benzene were the main BTX, while Acenaphthene, Fluorene, and Pyrene were the main PAHs. Concentrations of BTX/PAHs were negatively correlated with altitude, revealing altitude might be an important geological factor influencing spatial distribution of BTX/PAHs. PMF model demonstrated that the BTX/PAHs pollution in RA mainly originated from coking industrial activities. Health risk assessments were conducted by a modified US EPA-based model, in which

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environmental concentrations were replaced by residual concentrations after boiling. Residual ratios of different BTX/PAHs were determined by boiling experiments to be 9.4–93.8 %. The average total carcinogenic risks after boiling were decreased from 2.6×10^{-6} to 1.4×10^{-6} for adults, and from 4.3×10^{-6} to 2.1×10^{-6} for children, suggesting boiling was an effective strategy to reduce the carcinogenic risks from BTX/PAHs, especially for ingestion pathway. Monte Carlo simulation results matched well with the calculated results, suggesting the uncertainty was acceptable and the risk assessment results were reliable. This study provided useful information for revealing the spatial distribution of BTX/PAHs in underground drinking water of coking contaminated sites, understanding their linkage with altitude, and also helped to more accurately evaluate the health risks by using the newly established boiling-modified models.

1. Introduction

Coke is one of the most important energy fuels for industrial production, which holds an significant position in worldwide energy structure (Li et al., 2019). According to the U.S. Energy Information Administration, global coke production in 2021 reaches 706 million tons (www.eia.gov), while the coke production of China is 464 million tons (www.stats.gov.cn), accounting for 65.7 % of the global coke production. Accompanied with the development of coking industry, there are large amounts of coking contaminated sites in China (Li et al., 2023b), especially in Shanxi Province, which contributes 21.2 % of the total coke production. During coke production, large quantities of wastewater, exhaust gas and solid waste could discharge into the air/water/soil environment, leading to deterioration of ecological system and posing threats to human health (Zhang et al., 2019; Xu et al., 2021).

Benzene series including benzene, toluene and xylene (BTX), as well as polycyclic aromatic hydrocarbons (PAHs) have been reported to be characteristic pollutants discharged from coking industry (Mu et al., 2023; Zhang et al., 2023b). Zhang et al. (2020) had found that alkanes and olefins were the main pollutant in air during coke production, leading to atmospheric pollution in the region. Cao et al. (2022) measured the concentration of 16 PAHs in the surface soil of coking contaminated sites and found that 16 PAHs in the soil pose a definite carcinogenic risk to human. However, water pollution is relatively limited. Jiang et al. (2022) analyzed the occurrence of 16 PAHs in groundwater and evaluated potential ecological risks. The concentration of 16 PAHs was found to be between 15.04 and 449.13 ng/L, posing a moderate ecological risk to the local aquatic environment. Additionally, we have previously identified VOCs in coking wastewater and found VOCs in regulating tank can pose definite risk to human (Wang et al., 2023). These organic pollutants can migrate to groundwater through dry and wet sedimentation or surface runoff, thus causing groundwater pollution (Sarria-Villa et al., 2016; Chen et al., 2018). It has been reported that PFCS-containing wastewater and sludge from industrialized areas could be discharged directly into receiving water bodies or used as fertilizers in agricultural fields, leading to soil and groundwater contamination (Castiglioni et al., 2015). Groundwater pollution and its associated human health risk assessment are important global issues, which have attracted ever increasing widespread concerns (Cao et al., 2023; Siegel et al., 2023; Xiao et al., 2023). According to United Nations (2022), 50 % of the world's domestic water supply relies on groundwater. In China, groundwater serves as the drinking water source of 70 % of China's population (Sun et al., 2023), especially in northwest China, where precipitation and surface water are limited (Zhu et al., 2019). However, the distribution characteristics of BTX and PAHs in groundwater of coking contaminated sites and the associated health risks to surrounding residents have not been well explored.

The spatial distribution profiles of pollutants in groundwater have been reported to be influenced by both natural and anthropogenic factors (Hao et al., 2018). Li et al. (2022) investigated 41 PAHs in water samples from the north of the Taihu Lake in China, and found that the distribution of PAHs in water was related to temperature. Salowsky et al. (2021) explored the occurrence of PAHs in groundwater of a gas plant near the Rhine River in Germany, and found that the concentration of pollutants decreased with increasing distance from the pollution source. Moreover, altitude as an important geographical factor, has been received increasing attention to shape the distribution profiles of pollutants. For instance, Sun et al. (2019) explored the connection between the vertical transfer of PAHs from soil to groundwater and altitude, and found that the concentration of PAHs in groundwater in low altitude areas (563–783 m) was related to altitude. However, few studies have been conducted on the impact of altitude to the pollutant distribution in groundwater of industrial contaminated sites. Thus, it is important to link the altitude with the spatial distribution of BTX and PAHs in ground drinking water of coking contaminated sites.

Moreover, current health risk assessment for drinking water mainly focuses on urban tap water and surface water (Hu et al., 2016; Cao et al., 2018), while the researches on underground drinking water around industrial contaminated sites are rather limited. The evaluation approaches for health risk assessment are often based on the models provided by U.S. Environmental Protection Agency (US EPA) (Wu et al., 2013; Chen et al., 2021b). In most of the studies, the environmental concentrations of pollutants are directly used as the final concentrations to assess the risks by the models (Ambade et al., 2021). In fact, drinking water are usually boiled before consumption, which may lead to the reduction of concentrations after boiling due to volatilization and degradation (Chen et al., 2021a). Therefore, direct estimation using environmental concentrations may overestimate human health risks. Liu et al. (2019) had set 40 % as the residual ratio of all the organic pollutants after boiling for risk assessments, but the residual ratio (40 %) was only based on assumptions rather than measurements. In addition, the residual ratios would not be the same for different BTX and PAHs. Therefore, it is urgent to explore the real residual ratio of each BTX and PAHs after boiling to modify the EPA-based model by replacing the environmental concentrations with the residual concentrations after boiling. Thus, more accurate assessments of health risks for underground drinking water can be attained. However, due to the unavoidable uncertainty in health risk assessment, this may lead to unreliable results (Zhu et al., 2022). In this regard, Monte Carlo simulation is an effective probabilistic method that considers the uncertainty and sensitivity of different exposure pathways, thus providing more realistic risk assessments (Zhao et al., 2022). However, few studies have conducted on uncertainty analysis in assessing health risks of underground drinking water in coking contaminated sites.

Herein, the occurrence and risks of BTX and PAHs in underground drinking water of a typical coking contaminated site in Shanxi Province of China was systematically studied. The spatial distribution profiles of the BTX and PAHs were revealed with discussions on the linkage with altitude characteristics in this region. PMF model was used to identify the sources of PAHs in the underground drinking water in surrounding residential areas. Residual ratios of different BTX and PAHs were determined by boiling experiments, and were used to modify the US EPA risk assessment models. The carcinogenic and non-carcinogenic risks of BTX and PAHs via ingestion and dermal exposure were evaluated by the modified models. This work could shed light on the impacts of coking industrial activities to the distribution and risks of BTX and PAHs in underground drinking water, and also helped to reveal whether boiling could be used as control strategies for health risk mitigation of BTX/

PAHs contaminated drinking water. To the best of our knowledge, this is the first study to reveal the linkage between the distribution characteristics of BTX/PAHs and the geological factor of altitude in coking contaminated sites, as well as to establish a new boiling-modified model to assess health risks from BTX/PAHs in underground drinking water.

2. Experiments and methods

2.1. Study area

The study area is located in the Taiyuan Basin with high altitude in the northeast and low altitude in the southwest (https://zrzyt.shanxi.gov.cn), while the studied coking plant is located at the lowest altitude in this region (See Fig. 2). The coking plant has been operating steadily for 15 years, mainly produce coke, crude benzene, ammonia, sulfur and other products. It was surrounded by rural villages, and groundwater was used as the source of drinking water for the residents. An area of 10 × 6 km surrounding the coking plant is selected as the studied surrounding residential area. Additionally, the area 80 km from the coking plant and not affected by industrial pollution is also selected as a control area to explore the impact of coking production activities on the surrounding underground drinking water. All the rural residents in the study area use the groundwater in wells for drinking and domestic consumption. According to the field survey, there are a large number of trucks transporting coal all year round. Therefore, besides industrial pollution, vehicle exhaust pollution may also occur in this area.

2.2. Sampling and analysis

BTX and PAHs samples were collected separately with 3 independent parallels at 25 sampling sites (Table S1). Thus, a total of 150 water samples were obtained for further analysis. Briefly, BTX and PAHs samples were collected in 40 mL amber glass vials and 1 L amber glass bottles, respectively, and stored at 4 °C until analysis. Gas chromatography-mass spectrometry (7890B—5977B GC–MS; Agilent Technologies Inc., USA) coupled with a purge and trap concentrator (Atomx TekLink, USA) and triple quadrupole gas chromatograph coupled with a mass spectrometer (7890B—7000C, Agilent, USA) determined the concentration of BTX and PAHs, respectively (Zhao et al., 2021; Wang et al., 2023). Quality assurance (QA) and quality control (QC) procedures were strictly implemented from field operations to the analytical process according to Ambade et al. (2022b). Detailed information such as sample collection process, instrument detection parameters, method recovery rate and detection limit are listed in Text S1 and Table S2. During the sampling process, the latitude, longitude and altitude of the sampling points were obtained by Ovital Map.

2.3. Health risk assessment

The US EPA recommended Multimedia Environment Pollutant Assessment System (MEPAS) was used for human health risk analysis (Cao et al., 2018). The health risks from two main exposure pathways, ingestion and dermal exposure pathway, were calculated in this study. The carcinogenic risk (CR) values of $<1.0 \times 10^{-6}$, 1.0×10^{-6}– 1.0×10^{-5}, 1.0×10^{-5}– 1.0×10^{-4}, and $> 1.0 \times 10^{-4}$, indicated negligible risk, possible risk, probable risk, and definite risk, respectively. The detailed calculation methods were shown in Test S2, and the parameters used in the EPA-based model were shown in Table S3.

To evaluate the health risks more accurately, the environmental concentration of each BTX/PAHs in the models was replaced by the residual concentration after boiling, which was obtained by the following Eq. (1):

$$C^* = C \times R \quad (1)$$

where C^* is the residual concentration of each pollutant in underground drinking water after boiling (μg/L), C is the measured environmental concentration of each pollutant in underground drinking water (μg/L), R is the residual ratio of each pollutant after boiling (%). The R was obtained by simulated boiling experiments. Briefly, the standard solution of BTX and PAHs with known concentration was added to ultra-pure water (C_1), which was heated and boiled after completely dissolving, and the residual concentration was measured after cooling (C_2). R was obtained by the following Eq. (2):

$$R = \frac{C_2}{C_1} \times 100\% \quad (2)$$

The details can be found in Test S3.

2.4. Data analysis

The PMF model, which had been widely used to analyze the sources of pollutants in the environment, was used to analyze the source of PAHs (Ambade et al., 2023). The detailed calculation procedures were given in Text S4. All data about BTX and PAHs were analyzed by Agilent® MSD Chemstation workstation. One-way ANOVA test was performed using SPSS 27.0 for Windows (IBM, USA). Surfer® 2021 was used to map the spatial distribution of BTX/PAHs. To verify the uncertainty related to the calculation procedure and exposure coefficients, Monte Carlo simulation was performed here using Crystal ball software (16.0), and 10,000 iterations were calculated. Images were generated using Microsoft® Office Excel 2016, Origin® 2021, and other software.

3. Results and discussion

3.1. Occurrence of BTX and PAHs in underground drinking water

A total of 5 BTX and 14 PAHs were detected in underground drinking water samples, among which the total concentrations of BTX and PAHs in CP were 7.36 μg/L and 436.40 ng/L, respectively. The average total concentration of BTX and PAHs in RA were 1.38 μg/L and 47.32 ng/L, respectively. While the total concentration of BTX and PAHs were 0.13 μg/L and 0.48 ng/L in control area (CA), respectively (Table S4). The total concentrations of both BTX and PAHs followed the order of CP > RA > CA (Fig. 1(a)), suggesting the coking activities could impact the pollution status of underground drinking water in surrounding areas. The BTX concentrations in CP were 5.3 times higher than in RA, and 56.6 times higher than in CA. The PAHs concentrations in CP were 9.2 times higher than in RA, and 909.2 times higher than in CA. For the pollution profiles of BTX, the Toluene (PhMe) and Benzene (BEN) were the major BTX in CP and RA, accounting for 53.9 % and 65.9 % of the total BTX concentration, respectively (Fig. 1(b)). Wen et al. (2024) also found that PhMe and BEN were the main BTX in atmosphere in the study area. Pollutants in atmosphere can be transported and deposited to the soil and subsequently into groundwater via soil infiltration (Zhang et al., 2021). The distribution of characteristic BTX in atmosphere and groundwater was the same. Therefore, it was proposed that atmospheric deposition might be an important pathway for the pollution of underground drinking water. For the pollution profiles of PAHs, Acenaphthene (ACE), Fluorene (FLU) and Pyrene (PYR) were found to the major PAHs in CP with a total contribution of 69.6 %. Similarly, ACE was also the dominant PAH in RA with a total contribution of 41.0 % (Fig. 1(b)). We had previously explored the distribution characteristics of PAHs in surface soils in the study area, and also found that the ACE, FLU and PYR dominated in the surface soils (Zhang et al., 2023a), suggesting soil seepage could also be an important pathway for the pollution of underground drinking water.

The PAHs were further categorized into low molecular weight (LMW-PAHs), medium molecular weight PAHs (MMW-PAHs), and high molecular weight PAHs (HMW-PAHs) according to previous study (Ambade et al., 2021). It can be seen from Fig. S1, the relative contribution of HMW-PAHs was the lowest in the study area, which is opposite

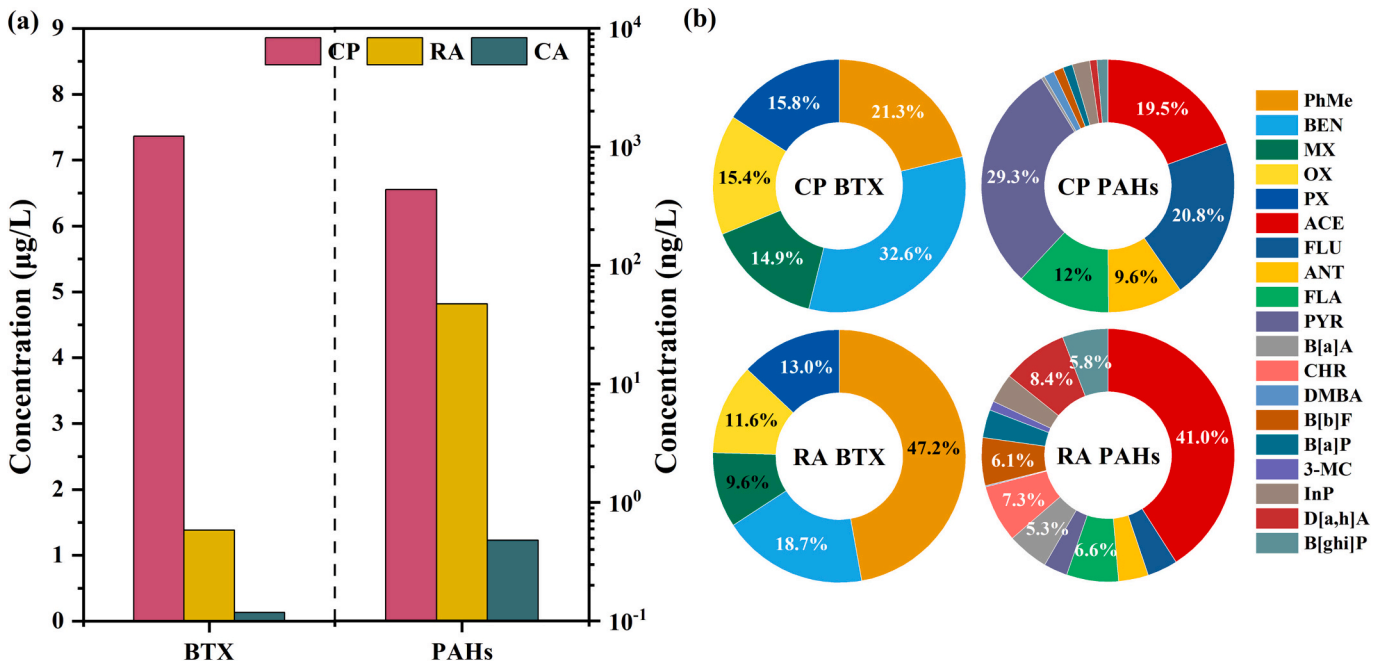

Fig. 1. Concentrations and relative contributions of BTX and PAHs in the study area: (a) concentrations of BTX and PAHs in coking plant (CP), residential area (RA) and control area (CA); (b) relative contribution of each BTX and PAHs in CP and RA. PhMe: Toluene; BEN: Benzene; MX: m-Xylene; OX: o-Xylene; PX: p-Xylene; ACE: Acenaphthene; FLU: Fluorene; ANT: Anthracene; FLA: Fluoranthene; PYR: Pyrene; B[*a*]A: Benzo(*a*)anthracene; CHR: Chrysene; DMBA: 7,12-Dimethlbenz[*a*]anthracene; B[*k*]F: Benzo(*k*)fluoranthene; B[*a*]P: Benzo(*a*)pyrene; 3-MC: 3-Methylcholanthrene; InP: Indeno(1,2,3-*cd*)pyrene; D[*a*,*h*]A: Dibenzo(*a*,*h*)anthracene; B[*ghi*]P: Benzo(*ghi*)perylene.

to the study of PAHs in the soil of industrial polluted area by Sankar et al. (2023). The relative contributions of HMW-PAHs in CP and RA were 3.7 % and 9.6 %, respectively. This was due to the fact that HMW-PAHs were poorly water soluble and tended to adsorb to soil or sediment, and thus were less likely to enter underground water (Duttagupta et al., 2020).

The concentrations of BTX/PAHs in this study were compared with other industrialized areas worldwide (Table 1 and Table 2). It showed that the concentration of BTX in underground drinking water in the study area was far less than gasoline-contaminated ground water in Stafford, New Jersey (Sanders and Hers, 2006), industrial pollution area in Eleusis, West Attica, Greece (Makri et al., 2020), fuel distribution station in Galicia, north-west Spain (Balseiro-Romero et al., 2016) as well as areas contaminated due to underground pipeline leaks in Chennai city, India (Rajasekhar et al., 2020). However, the concentration of PAHs in in the study area was higher than industrialized areas in Southern Jharkhand, India (Ambade and Sethi, 2021) and city area in Terai Belt, North India (Masih et al., 2014). And it was similar to the concentration of underground drinking water in coal mining areas in Anhui, China (Jiang et al., 2022), but much lower than polluted areas of the automobile industry in Merida city, Mexico (Rafael et al., 2019), fuel-impacted areas in Ado-Ekiti, Nigeria (Ibigbami et al., 2020), and coal mining area in Guangxi, China (Huang et al., 2016). These results indicated that BTX and PAHs pollution in the study area is at moderate level and PhMe, BEN, ACE, FLU and PYR are the major contaminants.

Table 1
Concentrations of total BTX in groundwater (μg/L) in selected sites worldwide.

Locations	Characteristic	Ranges	Mean	Reference
Stafford, New Jersey	Gasoline contaminated area	27–79,000	21,300	(Sanders and Hers, 2006)
Eleusis, West Attica, Greece	Industrial pollution area	ND – 95.0	27.4	(Makri et al., 2020)
Galicia, NW Spain	Fuel distribution station	4.9–425.8	8.97	(Balseiro-Romero et al., 2016)
North Chennai, India	Pipeline leaks area	33.4–17,817	541.3	(Rajasekhar et al., 2020)
Shanxi, China	Coking contaminated area	0.13–7.36	1.07	This study

Table 2
Concentrations of total PAHs in groundwater (ng/L) in selected sites worldwide.

Locations	Characteristic	Ranges	Mean	Reference
Southern Jharkhand, India	Industrialized area	6.4– 196.1	13.2	(Ambade and Sethi, 2021)
Terai Belt, North India	City area	10.24–43.85	21.0	(Masih et al., 2014)
Anhui huaibei, China	Coal mining area	15.0–449.1	104.8	(Jiang et al., 2022)
Merida City, Mexico	Automobile industry area	< LOD – 24,920	7233	(Rafael et al., 2019)
Ado-Ekiti, Nigeria	Fuel impacted area	404.0–6100.0	2530	(Ibigbami et al., 2020)
Guangxi, China	Coal mining area	257.6–495.5	381.2	(Huang et al., 2016)
Shanxi, China	Coking contaminated area	0.5– 436.4	19.1	This study

3.2. Spatial distribution and linkage with altitude

The spatial distribution characteristics of pollutants in underground drinking water were further explored. The contour map clearly showed that CP was the most polluted area with the highest concentrations of BTX/PAHs. In addition, the spatial distribution profiles of BTX and PAHs were similar in the study area (Fig. 2(a-b)), suggesting they might come from similar sources. Previous studies had shown that underground water generally flows from high altitude areas to low altitude areas, which might drive the distribution of organic matters in groundwater (Fels, 1999). Therefore, the linkage with altitude was further studied. The Pearson's correlation coefficients showed an important negative

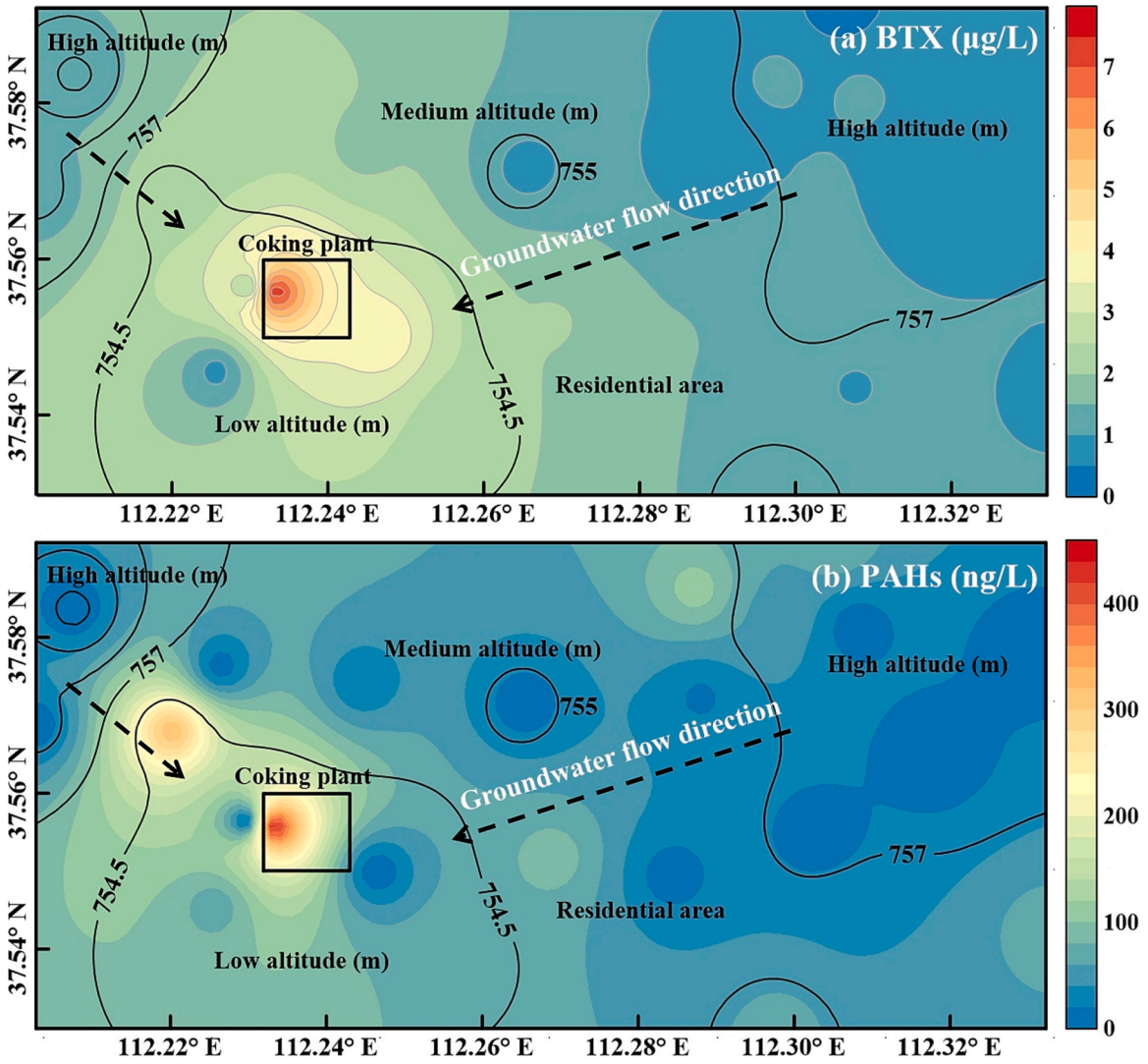

Fig. 2. Altitude distribution and concentration spatial distribution of BTX/PAHs in underground drinking water in the study area: (a) BTX; (b) PAHs.

correlation between the altitude of the sampling sites and the concentrations of BTX/PAHs ($p < 0.05$) (Table S5), suggesting high altitude was associated with low concentrations of BTX/PAHs. Therefore, the altitude of the sampling sites was analyzed in combination with the spatial distribution of concentrations (Fig. 2). According to inverse distance weighting, the study area was divided into high altitude area, medium altitude area and low altitude area (Guo et al., 2021). Fig. S2 further compared the BTX/PAHs concentrations at different altitudes. It confirmed that the concentrations of BTX in low altitude area were higher than that in medium altitude area and high altitude area (Fig. S2 (a)). Similarly, the concentrations of PAHs in low altitude area were significantly higher than that in medium altitude area and high altitude area (Fig. S2(b)). The concentrations of BTX and PAHs followed the order of low altitude area > medium altitude area > high altitude area. These results indicated that there were relationships between altitude and spatial distribution of BTX/PAHs, suggesting altitude might be an important geographical factor to shape the pollution profiles of underground drinking water.

Altitude exerts a multifaceted influence on the concentrations and spatial distribution of BTX and PAHs in groundwater. Several key mechanisms may come into play at varying elevations. Firstly, atmospheric deposition plays a crucial role, with higher altitudes experiencing different pollutant compositions due to air circulation patterns and emissions from various sources. These pollutants can be transported and deposited onto the ground and subsequently into groundwater, thereby affecting the composition and levels of BTX and PAHs. Secondly, temperature variation is inversely correlated with altitude, leading to lower temperatures at higher elevations. This temperature disparity can impact the solubility and volatility of BTX and PAHs, potentially making them less soluble in water and more prone to retention in solid phases or adsorption onto particles. Additionally, altitude can influence precipitation patterns, leading to variations in the amount and type of precipitation received at different elevations. This, in turn, can affect the transport and dilution of BTX and PAHs in groundwater, contributing to concentration variations across altitudes. Furthermore, altitude-related changes in soil characteristics, such as soil type and organic matter content, can influence the adsorption, degradation, and transport of these compounds in soil and groundwater. The geological and hydrogeological characteristics also vary with altitude, influencing the movement and flow direction of groundwater and contributing to variations in the spatial distribution of BTX and PAHs. Moreover, altitude-related shifts in vegetation and microbial communities can impact microbial degradation processes, which play a significant role in removing these contaminants from groundwater. Lastly, human activities, including industrial processes and agriculture, may differ in intensity and presence at varying altitudes, potentially acting as sources of BTX and PAH contamination and further contributing to concentration differences in groundwater across altitude regions. These factors

collectively affect the composition and levels of BTX/PAHs, as well as their transport and distribution in groundwater. Thus, further research is still needed to fully understand the mechanisms underlying the linkage between altitude and pollution profiles of BTX/PAHs in underground drinking water.

3.3. Source analysis

EPA PMF 5.0 was used to analyze the sources of BTX/PAHs in underground drinking water samples in RA. The Q(Ture)/Q(Robust) ratio was used to determine the number of factors and the relative contributions of each potential source (Zhang et al., 2017). 6 factors were determined according to the minimal changes of Q(Ture)/Q(Robust) with the increase of the number of source factors (Fig. S3). And their relative contributions were 68.4 %, 2.4 %, 13.2 %, 2.1 %, 10.5 % and 3.4 %, respectively (Fig. 3(a)). The source profiles in the PMF results were shown in Fig. S4 and Table S6.

Fig. 3(b) show the correlation between different BTX/PAHs and the relative contribution to each factor. Factor 1 might have been associated with coal burning. This factor was characterized by PhMe (72.2 %), BEN (53.5 %), m-Xylene (MX, 72.6 %), o-Xylene (OX, 74.1 %), p-Xylene (PX, 71.6 %) and Anthracene (ANT, 68.1 %). There was a high correlation between these organic matters, which meant that their sources should be similar. It had been shown that PhMe, BEN, MX, OX and PX are the products of coal burning (Lee et al., 2018; Bian et al., 2022). Therefore, factor 1 was attributed to coal burning. Factor 2 was allocated to coking emission. It was mainly composed of Fluoranthene (FLA, 85.6 %), PYR (80.1 %), Chrysene (CHR, 72.5 %) and FLU (69.2 %). Studies had shown that FLU, FLA and PYR were the main components of coke oven emissions (Cvetković et al., 2015; Li et al., 2020). CHR can be considered as geochemical markers for identifying coal combustion (ChooChuay et al., 2022). Previous studies had shown that PYR and CHR were the indicators for coal burning (Ambade et al., 2022a). Therefore, factor 2 was attributed to coking emission. Factor 3 could be interpreted as petroleum leak. This factor was dominated by ACE (80.3 %) and FLU (24.6 %). Pongpiachan et al. (2018) reported that LMW-PAHs were widely detected in oil spill areas. It was reported that ACE and FLU are often associated with the petroleum leak (Sun et al., 2020). Therefore, it was inferred that factor 3 was petroleum leak. Factor 4 might be related to fossil burning. It was mainly composed of Dibenzo(*a*,*h*)anthracene (D[*a*,*h*]A, 75.6 %), Indeno(1,2,3-*cd*)pyrene (InP, 16.7 %) and Benzo(*ghi*)perylene (B[*ghi*]P, 16.9 %). Previous research had shown that D[*a*,*h*]A, BaP, B[*ghi*]P and InP were the indicator of diesel and gasoline combustion (Yang et al., 2021). It was reported that D[*a*,*h*]A belonged to a pyrolysis product, which was related to coal tar combustion in coking plant (Galvao et al., 2023) and iron and steel smelting process (Wang et al., 2020). Therefore, factor 4 was attributed to fossil burning. Factor 5 might have been associated with vehicle emission. This factor was mainly composed of InP (37.4 %), B[*ghi*]P (36.8 %) and Benzo(*a*)pyrene (B[*a*]P, 30.5 %). ChooChuay et al. (2020) also pointed out that InP and B[*ghi*]P were mainly derived from the combustion products of petroleum products, such as motor vehicles and petroleum combustion. Studies had shown that InP, B[*ghi*]P and B[*a*]P were mainly released from vehicles (Gong et al., 2022). Therefore, it was inferred that factor 5 was vehicle emission. Factor 6 was allocated to biomass burning. It was mainly composed of 3-Methylcholanthrene (3-MC, 72.6 %), 7,12-Dimethlbenz[*a*]anthracene (DMBA, 42.2 %) and Benzo(*b*)fluoranthene (B[*b*]F, 33.8 %). Studies had shown that 3-MC and DMBA were the pollutant generated by wood combustion (Taiwo et al., 2019). It was also proposed that B[*b*]F was a characteristic product emitted in the process of biomass combustion (Pongpiachan et al., 2022). Therefore, the factor 6 was determined to be biomass burning.

Source apportionment of BTX/PAHs in groundwater using PMF model has certain limitations and challenges, such as model uncertainty, source quantity assumptions, temporal variability, overfitting, nonlinear independence, and data quality impacts. Nevertheless, PMF is still a valuable tool that can be combined with other methods such as sensitivity analysis and context specificity to improve the robustness and reliability of its results. In summary, the six sources were coal burning, coking emission, petroleum leak, fossil burning, vehicle emission and biomass burning. It could be inferred that BTX/PAHs in RA mainly came from coal burning (68.4 %) (Fig. 3(a)), which was consistent with the results of the above inference. In addition, the proportion of vehicle emissions reached 10.5 %, which may be attributed to the presence of a large number of trucks engaged in coal transportation in RA near CP. In fact, gasoline or diesel fuel had a complex composition containing a large number of hydrocarbons, including aromatics, alkanes, olefins, etc., which may also be important in influencing the distribution of BTX/PAHs in RA. Overall, the BTX/PAHs pollution in the underground drinking water of RA were mainly derived from the coking industrial activities.

3.4. Human health risk assessment

3.4.1. Health risks caused by non-boiled underground drinking water

Health risks were further estimated based on oral ingestion and

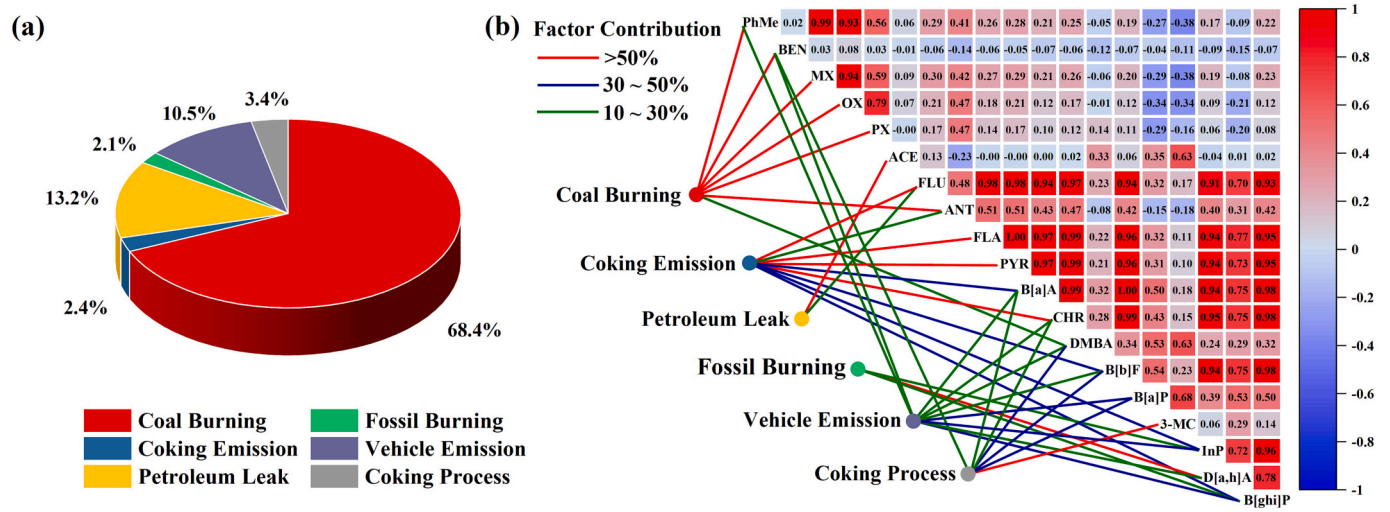

Fig. 3. Source apportionment by PMF model of BTX/PAHs in underground drinking water of residential area (RA): (a) relative contribution of 6 factors in PMF model; (b) correlation analysis between BTX/PAHs and their relative contributions to 6 factors.

dermal exposure pathways. The TCR for adults in CP, RA and CA were 5.1×10^{-5}, 2.6×10^{-6} and 2.9×10^{-7}, respectively. The TCR for children in CP, RA and CA were 9.7×10^{-5}, 4.3×10^{-6} and 5.1×10^{-7}, respectively (Table S7). It was obvious that the carcinogenic risk for children was higher than that for adults, indicating that children were more vulnerable to carcinogenic risk from BTX/PAHs than adults. The carcinogenic risks followed the order of CP > RA > CA (Table S7). In CP, both adults and children were at probable risk (10^{-5}– 10^{-4}). In RA, 43.5 % of adults were at negligible risk ($<10^{-6}$), with 56.5 % were at possible risk (10^{-6}– 10^{-5}), and 39.1 % of children were at negligible risk, with 47.8 % were at possible risk and 13.1 % at probable risk (calculated by ratio of sampling points, Table S8). In contrast, both adults and children were at negligible risk ($<10^{-6}$) in CA, which indicated that the carcinogenic risk of BTX/PAHs in underground drinking water in CP and RA would be increased due to the influence of coking industrial activities. It was worth noting that the carcinogenic risks caused by 3-MC and DBMA in RA exceed the risk threshold (10^{-6}) (Fig. 4(a)). However, 3-MC and DMBA were not belong to the 16 priority control PAHs. Attention should be paid to the two PAHs due to the hazard to human. For non-carcinogenic risk, the HI for both adults and children from BTX/PAHs were below the risk threshold (HI <1) (Fig. 4(b)). This means adults and children in the study area would not receive a non-carcinogenic risk.

3.4.2. *Health risks caused by boiled underground drinking water*

Subsequently, the health risks were assessed using the modified model considering boiled drinking water. The residual ratios of different BTX/PAHs were determined by boiling experiments to be 9.4–93.8 %. The TCR for adults in CP, RA and CA were 9.1×10^{-6}, 1.4×10^{-6} and 2.0×10^{-7}, respectively. The TCR for children in CP, RA and CA were 1.6×10^{-5}, 2.1×10^{-6} and 3.4×10^{-7}, respectively (Table S7). After boiling, the carcinogenic risk for adults in CP decreased from probable risk (10^{-5}– 10^{-4}) to possible risk (10^{-6}– 10^{-5}). And for children, the TCR was still at probable risk (10^{-5}– 10^{-4}), but it significantly decreased by 83.5 %. As for RA, the proportion of adults at negligible risk ($< 10^{-6}$) increased from 43.5 % to 52.2 %, the proportion of children at negligible risk increased from 39.1 % to 43.5 %, with the proportion of children at possible risk (10^{-6}– 10^{-5}) increased from 47.8 % to 56.5 %, and the proportion of children at probable risk decreased from 13.1 % to 0.0 % (calculated by ratio of sampling points, Table S8). Similarly, the carcinogenic risks for adults and children in CA were also significantly reduced by 45.0 % and 33.3 %, respectively (Table S7). Moreover, the carcinogenic risks for 3-MC and DMBA in CP significantly decreased by 37.1 % and 56.4 % (Fig. 4(c)). This difference was due to the fact that the carcinogenic risks of 3-MC was mainly due to the dermal expose, whereas the carcinogenic risk for DMBA was mainly due to the ingestion (Fig. S5). Boiling significantly reduced the concentration of orally ingested organic pollutants. Thus, the carcinogenic risk for DMBA was reduced to a greater extent than that of 3-MC. For non-carcinogenic risk, there were certain reduction after boiling to human (Fig. 4(d)). It also does not pose a non-carcinogenic risk to adults and children within the study area.

The carcinogenic risks via ingestion and dermal exposure pathways before and after boiling were compared to further reveal the effect of boiling on the health risk mitigation (Fig. 5). In the case of non-boiled underground drinking water, the carcinogenic risks were mainly from ingestion pathway, with a relative contribution of 41.3 % ~ 96.8 % and a mean value of 63.0 %. In contrast, the carcinogenic risks for boiled drinking water were mainly from the dermal exposure pathway, with a relative contribution of 18.2 % ~ 85.5 % and a mean value of 60.0 %. However, many studies ignore the carcinogenic risk caused by dermal exposure. Weschler et al. (2015) also pointed out that dermal exposure was an important pathway for organic pollutants to pose carcinogenic risks to human. Therefore, fully understanding of the carcinogenic risks caused by different exposure pathways of organic pollutants could

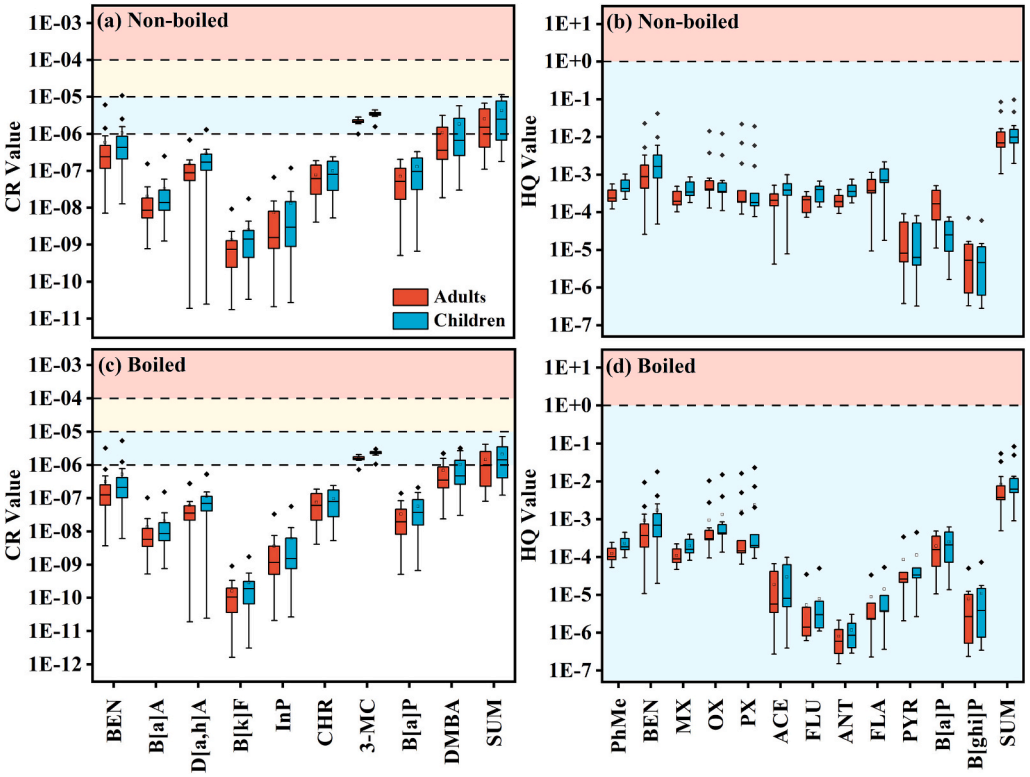

Fig. 4. Health risk assessment of underground drinking water for adults and children: (a) carcinogenic risk assessment; (b) non-carcinogenic risk assessment of non-boiled water; (c) carcinogenic risk assessment; (d) non-carcinogenic risk assessment of boiled water. The white, blue, yellow and red areas in (a) and (c) represent negligible risk (CR < 10^{-6}), possible risk (10^{-6} < CR < 10^{-5}), probable risk (10^{-5} < CR < 10^{-4}) and definite risk (CR > 10^{-4}) in carcinogenic risk, respectively. The blue and red areas in (b) and (d) represent negligible risk (HQ < 1) and definite risk (HQ > 1) in non-carcinogenic risk.

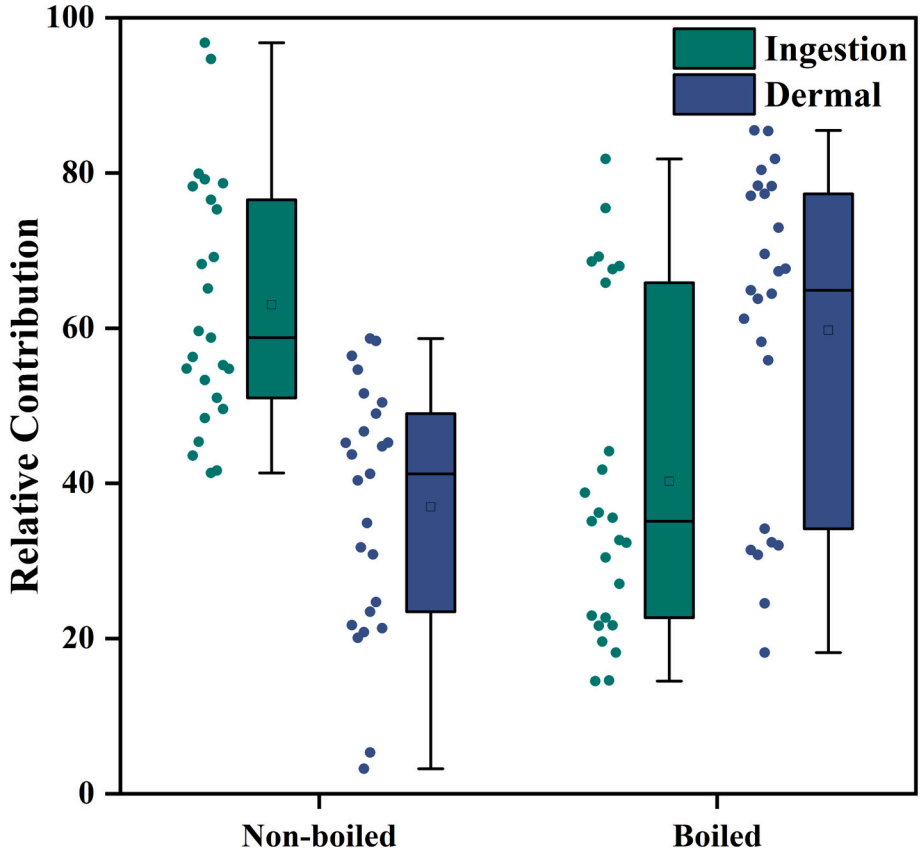

Fig. 5. Comparison of the relative contribution of total carcinogenic risk via ingestion and dermal exposure pathways from underground drinking water before and after boiling.

effectively prepare preventive measures. Underground drinking water were usually boiled before consumption, which might reduce the concentration of BTX/PAHs after boiling due to volatilization and degradation. Therefore, the carcinogenic risk caused by ingestion would be reduced (Liu et al., 2019). This result suggests boiling could significantly reduce the carcinogenic risks of BTX/PAHs via oral ingestion pathway.

The above results indicated that boiling significantly reduced the human health risk of BTX/PAHs in underground drinking water, suggesting that boiling was an effective strategy to reduce the carcinogenic risk of underground drinking water. Meanwhile, the carcinogenic risk from the dermal exposure pathway also needed to be concerned. Although the consumption of boiled underground drinking water reduced the total and non-carcinogenic risk, the carcinogenic risk of underground drinking water pollution caused by coking industrial

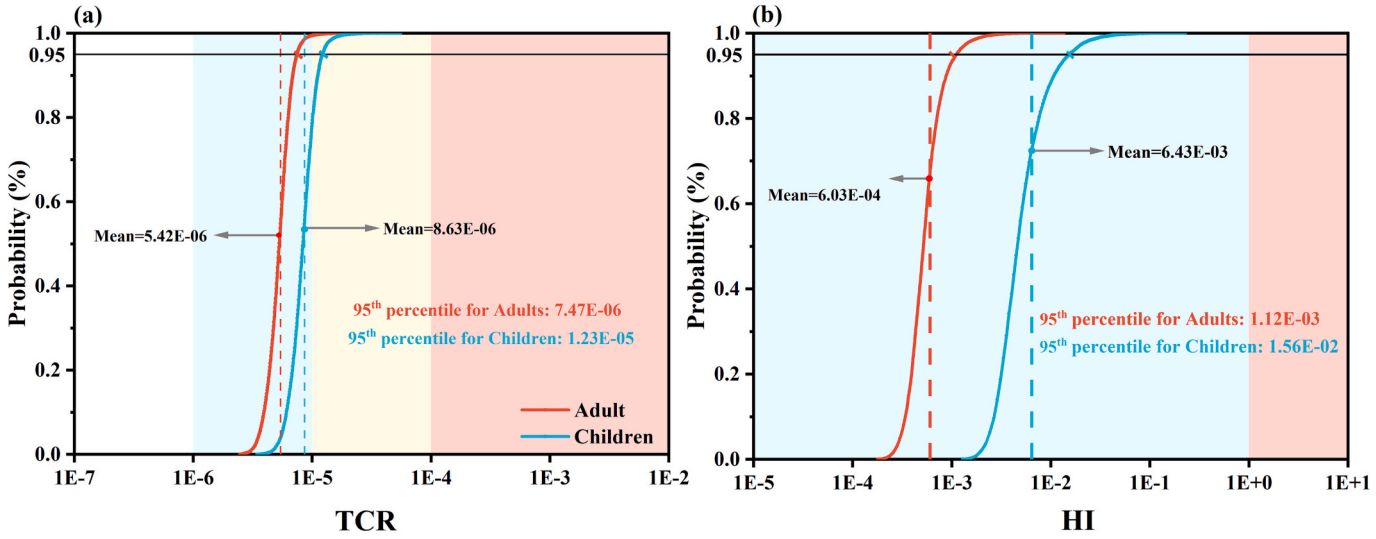

Fig. 6. Cumulative probabilistic estimate of total carcinogenic risk (a) and hazard index (b) of boiled underground drinking water. The white, blue, yellow and red areas in (a) represent negligible risk ($CR < 10^{-6}$), possible risk ($10^{-6} < CR < 10^{-5}$), probable risk ($10^{-5} < CR < 10^{-4}$) and definite risk ($CR > 10^{-4}$) in carcinogenic risk, respectively. The blue and red areas in (b) represent negligible risk ($HQ < 1$) and definite risk ($HQ > 1$) in non-carcinogenic risk.

activities was also of concern.

3.5. Monte Carlo simulations

3.5.1. Probabilistic risk assessment

In this study, 10,000 Monte Carlo simulations were performed. The cumulative probabilistic estimate of adults and children exposed to BTX/PAHs in boiled and non-boiled underground drinking water were simulated by Monte Carlo simulation and results were showed in Fig. 6 and Fig. S6, respectively. For boiled underground drinking water, the probabilistic TCR ranged from 2.5×10^{-6} to 3.5×10^{-5} with a mean value of 5.4×10^{-6} for adults, and from 3.4×10^{-6} to 5.5×10^{-5} with a mean value of 8.4×10^{-6} for children (Fig. 6(a)). Overall, 0.5 % of TCR exceeded 10^{-5} for adults, and 21.4 % of TCR exceeded 10^{-5} for children. It confirmed that both adults and children suffered carcinogenic risk in RA. This result was consistent with the health risk assessment. While Fig. 6(b) showed the probabilistic HI of BTX/PAHs for adults and children. The probabilistic HI ranged from 1.8×10^{-4} to 1.4×10^{-2} with a mean value of 6.0×10^{-4} for adults, and from 1.3×10^{-3} to 2.3×10^{-1} with a mean value of 6.4×10^{-3} for children. It indicated that both adults and children are not at risk of non- carcinogenic, which was consistent with calculation results. To sum up, the results suggested that the parameters of health risk assessment in this study were reasonable and the results were reliable.

However, the use of Monte Carlo simulation for health risk assessment of BTX/PAHs in boiled and non-boiled underground drinking water still faces limitations. Firstly, it relies on comprehensive and precise data encompassing BTX/PAHs concentrations, consumption patterns, exposure durations, and toxicological parameters, which may be challenging to obtain, potentially introducing uncertainties into the modeling process (Li et al., 2023a). Secondly, the accuracy of Monte Carlo simulations heavily depends on assumptions made about exposure parameters and dose-response relationships. Small variations in these assumptions can lead to significant fluctuations in estimated exposures and associated risks, rendering the results sensitive to modeling choices.

3.5.2. Sensitivity analysis

The sensitivity of variables to TCR and HI for adults and children were analyzed together with Monte Carlo simulation (Fig. S7). Among the parameters, EF (exposure frequency) contributed the most to the total variance of TCR, which accounted for 73.9 % and 67.8 % for adults and children, respectively. ED (exposure duration) contributed the second highest to total variance of TCR (30.0 % for adults and 27.1 % for children), followed by IR (water ingestion rate) (25.4 % for adults and 27.4 % for children). For non-carcinogenic risk, EF, ED and IR also remain the three parameters with relatively high contribution. The relative contributions of EF, ED and IR for adults and children were 72.7 %, 29.7 %, 38.5 %, and 66.5 %, 26.5 %, 37.6 %, respectively. Whereas BW had a very strong negative contribution rate to both TCR and HI for adults (−30.8 %, −46.1 %) and children (−29.8 %, −44.9 %), respectively, which further explained why children suffered higher health risks than adults.

3.5.3. Uncertainty analysis

Uncertainty exists in human health risk assessment. Firstly, the availability of toxicological data for both BTX and PAHs is limited, potentially necessitating the use of assumptions or data extrapolation, which can introduce uncertainties (Li et al., 2016). Secondly, Monte Carlo simulations assume that exposure to different compounds is independent, although in reality, some BTX/PAH compounds may have shared sources or similar exposure pathways, leading to potential inaccuracies in risk estimates. The complexity of exposure pathways for BTX/PAHs, including factors like boiling water and the potential for changing human behaviors over time, adds further uncertainties. Thirdly, the parameters values are directly derived from the recommended values of USEPA (USEPA, 2011), which are not totally suitable for peoples living in different countries. Thus, alternative assessment frameworks are still needed for local conditions in future works. Finally, interpreting the results and effectively communicating probabilistic risk estimates to stakeholders and decision-makers can be complex, requiring specialized expertise. Overall, while Monte Carlo simulation is a powerful tool for probabilistic risk assessment, its application to BTX/PAH exposure estimation in underground drinking water entails various complexities and challenges that necessitate careful consideration and validation for reliable results.

4. Conclusions

In summary, the distribution characteristics, sources, and health risk of BTX and PAHs in underground drinking water at a typical coking contaminated site were investigated. The average concentrations of BTX and PAHs in underground drinking water of the coking plant were 5.1 and 4.8 times higher than those in the residential areas, respectively. PhMe, BEN ACE, FLU and PYR were the characteristic pollutants. Moreover, the concentrations of BTX/PAHs were negatively correlated with altitude, revealing that altitude might be also an important factor influencing the distribution of BTX and PAHs. Source analysis showed that BTX/PAHs in the residential area were mainly from coking industrial production activities, which posed a certain carcinogenic risk to human. Additionally, the health risk assessment was revised by applying the residual ratios of BTX/PAHs after boiling. Residual ratios of different BTX/PAHs were determined by boiling experiments to be 9.4–93.8 %. And the results showed that the concentrations of BTX/PAHs in underground drinking water were reduced to different degrees after boiling. Therefore, boiling was revealed to be an effective strategy to abate the health risks of BTX/PAHs. Additionally, Monte Carlo simulations had verified the accuracy of health risk assessment, the proportion of adults at carcinogenic risk ($> 10^{-6}$) were 47.8 %, with the proportion of children were 56.5 %. These findings revealed the serious impact of coking industry activities on the underground drinking water of surrounding residential environment. They were helpful to understand the linkage between BTX/PAHs distribution and altitude, and to more accurately evaluate the health risks by using the boiling-modified models.

CRediT authorship contribution statement

Wanjun Wang: Conceptualization, Funding acquisition, Project administration, Writing – review & editing. **Shaobin Shao:** Formal analysis, Investigation, Visualization. **Weiqiang Deng:** Methodology, Software. **Congqing Wang:** Investigation, Visualization. **Xinyuan Liu:** Data curation, Validation. **Hailing Li:** Formal analysis, Methodology. **Meicheng Wen:** Investigation, Visualization. **Xin Zhang:** Resources, Validation. **Guiying Li:** Data curation, Investigation. **Taicheng An:** Conceptualization, Funding acquisition, Resources.

Declaration of competing interest

Wanjun Wang reports financial support was provided by National Key Research and Development Program of China. Wanjun Wang reports financial support was provided by National Natural Science Foundation of China. Wanjun Wang reports financial support was provided by Guangdong Basic and Applied Basic Research Foundation. Wanjun Wang reports financial support was provided by Key Research and Development Program of Guangdong Province. Taicheng An reports financial support was provided by Local Innovative and Research Teams Project of Guangdong Pearl River Talents Program. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2024.170407.

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