Research Paper





Measuring 1, 3-Butadiene and Simulation of its Releasing Method by GIS Application and Cancer Risk Assessment in Tehran in 2019-2020

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ABSTRACT

Background: According to the heavy traffic in Tehran, a high amount of 1, 3-Butadiene (BD) in this city is highly expected. This study estimated the lifetime cancer risk (LCR) attributable to BD in District 9 of Tehran Municipality and simulation of its releasing way.

Methods: This research is an applied study that was conducted in the form of field research. Cancer risk assessment was carried out based on the United States Environmental Protection Agency (USEPA) method. BD concentration measurements were performed at 30 points and specified in the area and daily at three different times in four seasons since autumn of 2019 till summer of 2020. LCR then was calculated for four different groups of residents, employees, first and second classes of the pedestrian. Finally, the way of releasing BD in the District 9 was evaluated by GIS software.

Results: The results showed that the highest and lowest BD concentrations were 2819 and 424 ppb, respectively, in autumn and spring. They were measured in the north and west side of the District 9 which were much higher than inhalation reference concentration. In addition, the LCR estimation of population due to exposure to high level of BD was exceeded the USEPA benchmark of 1×10^{-6} in the 4 specified groups. So, the amount of LCR in the residents was 790 times more than the USEPA benchmark.

Conclusion: According to the results, the necessity for traffic control by urban management and producing green vehicles to prevent pollutants emission is essential.

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1. Introduction

uel consumption and traffic volume can pollute the air in big cities. This pollution is mostly formed by fuel combustion, and it enters the atmosphere in the form of pollutant gas or particles. According to the emitting resources, the air pollutant is divided into two groups of fix and mobile. As its name suggests, the fixed group includes industries, power stations, residential and commercial centers, and mobile resources consist of different types of vehicles, from motorcycles to airplanes and boats [1].

1, 3-Butadiene is classified as a carcinogenic compound (Code C29790, National Cancer Institute) [2] or Group 1 carcinogen by International Agency for Research on Cancer [3]. Even though 1, 3-Butadiene is easily decomposed in the air, and there are still noticeable levels in many urbanized cities, especially in dense traffic and industrial areas. Despite of its toxicity, 1, 3-Butadiene is one of the main materials for polymer industries, i.e., rubber, plastic, and other chemical industries, posing higher risk to the workers. Major sources of 1, 3-Butadiene are listed as combustion activities, including mobile vehicle exhaust, industrial activities, forest fires, and leaks from ships and industrial facilities [4]. Inhalation is considered as the major pathway of 1, 3-Butadiene to the human body. Inconsiderable amount of this contaminant is exposed through dermal contact and digestion pathway, even though detected levels have been found in some plastic food containers [5]. Acute exposure to 1, 3-Butadiene cause's eyes, nasal passage, lung, and throat irritations. It can cause headache, fatigue, decreased blood pressure and pulse rate, central nervous system damage and unconsciousness at high 1, 3-Butadiene level exposure. Dermal exposure to 1, 3-Butadiene also causes frostbite [6]. The chronic effects due to 1, 3-Butadiene exposure, i.e., cancer and cardiovascular system diseases, have been the controversial issues. Some factors such as cigarette smoke and other toxicants (i.e., benzene and styrene) may confound the true chronic effects caused by 1, 3-Butadiene exposure [6]. However, 1, 3-Butadiene is a carcinogenic agent, which was reported to cause Deoxyribonucleic Acid (DNA) damage [7, 8]. This toxicant metabolically activates the genotoxic epoxides, resulting in abnormality in DNA adducts and chromosomes [9].

One of the most important metabolites of 1, 3-Butadiene is Di Epoxy Butane (DEB) which causes DNA damage by producing reactive oxygen species (ROS) and 8-OHdG [10]. 1, 3-Butadiene is highly reactive and can be transformed to more toxic pollutants under the pho-

tochemical reactions [11]. Despite of its toxic properties, 1, 3-Butadiene is commercially produced for polymer industries in the world. It is used as the raw materials in many industries, for example, tires, car sealants, plastic bottles, and food wrap facilities [12].

1, 3-Butadiene is an industrial chemical material used for producing synthetic rubber as a monomer. This molecule can be as a two-group of attached vinyl CH2=CH2. The word "Butadiene" is usually used for 1, 3-Butadiene [13]. 1, 3-Butadiene is a colorless gas and has a slight smell like gasoline. The odor threshold for this compound is 1.6 ppm, and its molecular weight is 54.09 g/mol. The vapor pressure of it is 2100 mmHg in 25°C [14].

Personal exposure to the air contaminants reflects better the impacts of daily human activities of both indoor and outdoor environments than exposure to separate microenvironment [15]. There have been few studies that estimated the cancer risk caused by exposing to 1, 3-Butadiene personally.

In Europe, the available studies associated with 1, 3-Butadiene personal exposure were found in the United Kingdom and Sweden. In the United Kingdom, higher levels of 1, 3-Butadiene personal inhalation were found during daytime (average 1.1 μ g/m³ and max 26.3 μ g/m³), which were higher than those during nighttime (0.8 µg/ m³ and max 7.9 μg/m³) in Birmingham during 1999-2000 [16]. Similarly, Harrison et al. measured the personal exposure to 1, 3-Butadiene in four cities in the United Kingdom, categorizing into urban areas (i.e., London and Birmingham), suburban areas (i.e., Birmingham), and rural areas (i.e., West Midlands and Wales). The high concentration of 1, 3- Butadiene was found in urban Birmingham (0.56 µg/m³ and max 5.95 µg/m³), followed by rural West Midlands (0.51 µg/m³ and max 4.03 µg/ m³), suburban Birmingham (0.37 μg/m³ and max 6.27 $\mu g/m^3$), rural Wales (0.24 $\mu g/m^3$ and max 1.85 $\mu g/m^3$) and the lowest level was observed in urban London (0.1 $\mu g/m^3$ and max 0.76 $\mu g/m^3$).

Due to the four-city coverage and up-to-date data, the results reported by Harrison et al. were used to estimate the cancer risk assessment in the current study. In Sweden, four studies were associated with the 1, 3-Butadiene personal exposure [17]. The first two studies, i.e., Krusa et al. and Yazar et al., were conducted in Stockholm in 2002 and 2009, respectively. There were no significantly different results between two studies (0.7 vs. 0.5 $\mu g/m^3$ for average values and 3.1 vs. 2.3 $\mu g/m^3$ for max values) [18, 19]. Gustafson et al. compared the

1, 3-Butadiene personal exposure levels in two different environments, i.e., homes with wood burners (0.33 μg/m³) and without wood burners (0.14 μg/m³) in Hagfors, Sweden [20]. The study by Hagenbjork-Gustafsson et al. had the most comprehensive data because it was conducted in 5 cities of Sweden [21]. In Japan, Laowagul and Yoshizumi monitored the ambient levels of 1, 3-Butadiene at two sites in Tokyo, i.e., 0.49 μg/m³ for Shirogane and 0.91 μg/m³ for Hachimanyama [22]. By using data available at monitoring station in Tokyo, Mita et al. mentioned that 1, 3-Butadiene levels over the city were 0.064 μg/m³ [23].

The possibility of a high level of 1, 3-Butadiene presence in Tehran's air is highly expected because of following reasons: the principal resources of 1, 3-Butadiene emission in the air are vehicles' exhaust and rubbers and plastic production industries; furthermore, one of the major issues of Tehran is daily traffic of a large number of vehicles that cause heavy traffic and air pollution. Several rubber manufacturing companies around Tehran can increase the concentration of this material. Hence, this study aimed to evaluate and measure the level of 1, 3-Butadiene concentration and assess the risk of cancer in associated people living in Tehran's District 9. Although 1, 3- Butadiene contaminant is proved to pose cancer development, the cancer risk assessment has not been adequately studied. Several studies have conducted the experiments to quantify the concentrations of 1, 3-Butadiene by personal exposure or in various microenvironments; however, few studies focus on assessing cancer risk by exposing to this contaminant. To our best of knowledge, to date, no research has been done on the release of volatile organic compounds in urban areas, as well as in the field of risk assessment due to the release of such pollutants in different seasons of the year and in the whole area, which is one of the research innovations.

2. Materials and Methods

By investigating all 22 districts of Tehran, we concluded that the District 9 is the best zone for performing this research because most of the industrial factories are located in the west side of Tehran; also, there is heavy traffic of vehicles in Azadi square because of the West Terminal, buses park and ride, and Mehrabad Airfield. In this study, 30 points were selected from District 9 of Tehran and, at each point, 1, 3-Butadiene was measured three times during each season. A total of 360 measurements were taken. The measurements were made from direct readings with a portable device. In this research, a method was needed to measure 1, 3-Butadiene in the air of the District 9 of Tehran. These types of measure-

ments are performed by directly reading the concentration of the 1, 3-Butadiene or by device analysis such as gas chromatography. According to the district condition and the concentration of the Butadiene gas in the air, sampling and measuring method was performed by Phocheck 5000+, which is a direct reading approach. The measurements were performed three times in a different period of times during the week (at the beginning, middle, and end of the week) at certain points at four seasons of the year. Also, ten points were specified to determine the 1, 3-Butadiene concentration by personal sampling pump SKC and Carbone adsorbent 226-09.

According to the results of the measured 10 samples by adsorbents, the measured values by Phocheck 5000+ device were corrected and calibrated. Analyzing the results was performed by the SPSS v. 24 application. Zoning the releasing method of Butadiene gas from emitting centers in Tehran's air was done by GIS10 application. In this research, the risk assessment was performed for District 9's residents of District 9. In the risk assessment of this research, the residents, first and second classes of pedestrians and employees had the most contact with pollutants, so the effect of pollutants on these people's health was studied. The risk assessment process is performed for 1, 3-Butadiene. This monitoring determines these pollutants concentration in the air of the District 9 and investigates the exposure of residents, employees, and pedestrians of this district to these pollutants through the respiratory system. Thirty points were considered to be proper for sampling in Tehran's District 9. The 1, 3-Butadiene measurements were performed in different daytime and warm and cold seasons and also in different climate conditions.

After determining the 1, 3-Butadiene concentration in the air of various points of Tehran's District 9, the concentrations of these dangerous materials in the air that each citizen of Tehran is in contact with those in different ways were detected. The level of contact through the respiratory system will be separately measured and specified [24].

Then, the statistical results of 1, 3-butadiene measurements were analyzed. Friedman test was used in the statistical discussion due to the presence of one variable (1, 3-Butadiene) and several groups (seasons). Descriptive statistics of the research were also calculated. The informational system of IRIS has provided some factors such as average lifetime, mean weight, absorption coefficient, and time of contact during comprehensive investigations. By using these factors, we can specify that how much air each citizen of Tehran

in the District 9 inhale on average and how much 1, 3-Butadiene enters their body by measuring the pollutants concentrations in the air. After determining each citizen's final time of contact with any type of the mentioned pollutants, the increased risk of cancer associated with any of these materials will be measured and evaluated by reference dose (RFD) and inhalation reference concentration (RFC) factors [25]. In addition to cancer, the risk index was measured and determined for all materials with non-carcinogenic complications due to poor hygiene [13]. According to the results and daily contact of Tehran's population with heavy metals in the mentioned zone under the monitoring, the increased number of cancer in the lifetime of Tehran's citizens in the mentioned district was calculated quantitatively.

The suggested equations by the Risk Assessment Information System (RAIS) are used to determine Chronic daily Inhalation (CDI). These equations consider the humans' exposure to each of the existing pollutants in the air separately. Calculating the CDI for air pollutants in the residents of mentioned district associated with carcinogenic complications for the respiratory system is performed by Equation 1 [25]:

1.
$$CD_{stu-air-c}(\mu g/(m^3))$$

 $\frac{C_{aiv}(\mu g/m^3) \times EF(day/year) \times ED(year) \times ET(hours/day) \times (1day/(24hours))}{AT \{365(days/(year) \times LT(year)\}}$

The represents the amount of daily received pollutants due to the breathing.

The $CD_{\text{stu-air-c}}$ represents the pollutant concentration in the air in $\mu g/m^3$.

The EF represents exposure frequency in day/year.

The ED represents exposure dosage in year.

The ET represents exposure time in hour/day.

The LT³ represents lifetime in a year (70 years).

The AT represents the person's lifetime, which its risk calculation is equivalent to 70 years (average of a total lifetime) for carcinogenic diseases, and exposure time for non-carcinogenic diseases.

After estimating the carcinogenic CDI, the risk index will be calculated. The Lifetime Cancer Risk (LCR), described as the probability to get cancer caused by toxicant exposure, is the product of CDI and PF, as follows:

Two Equations 2 and 3 forms the base of calculations in this part [26]:

2. CR=CDI×SFOrIUR

, where the represents the possibility of developing cancer incidence in a person's lifetime (without a unit).

The CDI represents chronic daily intake or dose in pollutant weight/ air volume unit, such as mg/m³ [26].

3. The SF represents the incline coefficient of cancer in. 1/CDI unit

The IUR represents the unit risk for breathing in 1/CDI unit [26].

The area of study

This area is approximately 19.6 km², and its population is 174239 persons (57688 families), which includes 88163 men and 86076 women based on the census of the year 2017. Most of them were residents in Hashemi, Shamshiri, Shaheed Dastgheyb, Mehrabad, and Jey Street sectors. This area is restricted in the north by Azadi Street and the particular road for Karaj, and in the south by Fath highway and 45M Zarand, and in the east by Shahidan Street and Sadat Street, and in the west by Kan Creek. This area has two districts and eight neighborhoods in the urban restriction, and 47737 families are residents in these two districts. Figure 1 shows the position of Tehran the District 9 in relation to the city of Tehran and Iran country. There are important transportation roads in this study area.

Thirty points were selected for sampling in this area. These points were determined in this area's restriction. It covers all of the minor streets, major streets, highways, and gas stations.

3. Results and Discussion

The sampling was performed three times a day in the morning, noon, and night on measurement days. Table 1 shows the sampling results in the four seasons of the year separately in the form of averages.

Table 1 shows the results of the average measurement of 1, 3-Butadiene in District 9 of Tehran in the seasons of the year. These measurements were performed in 30 points of Tehran region. In some places, this value was very high. The reason is due to excessive car traffic and the presence of tall buildings, which increased the amount of pollutants and prevented air circulation at that point.

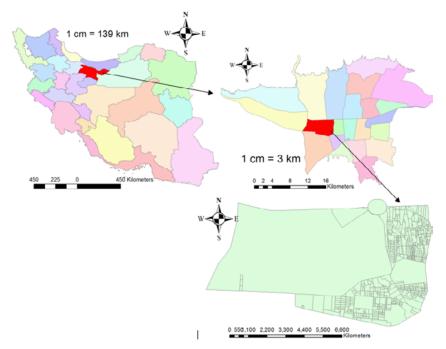


Figure 1. The area of study (District 9 of Tehran Municipality)

Table 2 shows the statistical analysis of the amount of 1, 3-Butadiene in the seasons of the year. This table shows descriptive statistics as well as a significant difference between the amounts of pollutants in the seasons.

The Friedman test was used to rank the release of 1, 3-Butadiene in the District 9 of Tehran. The test showed that the release rates of 1, 3-Butadiene were different in different seasons. Take a look at the column on the far right of this output table. It is the Asymptotic Significance, or P, of the chi-square run in SPSS. This value determines the statistical significance of the relationship tested. In all tests of significance, if P<0.05, we can say that there is a statistically significant relationship between the two variables. The p-value in our chi-square output was P=0.0001. This means that the relationship between 1 and 3 butadiene levels was significant in different seasons. Comparison of the mean results showed that the highest average emissions were in season, autumn, winter, summer and spring, respectively. The results of the differences and the significance of the results have been shown in Table 2.

Determining 1, 3-Butadiene emission in different seasons by GIS application

The GIS application helped the zoning of the amount of the 1, 3-Butadiene emission in four seasons of the year, which has been demonstrated in Figures 2-5. To evaluate the values of 1, 3-Butadiene in the District 9 of Tehran, the data should be entered into the GIS application. These data were stated in the form of the IDW model in the application environment.

Figure 2 shows the 1, 3-Butadiene emission zoning in the autumn season in the District 9 of Tehran. According to the sampling results, the highest level of 1, 3-Butadiene concentration in the autumn season was 2891 ppb. The southwest of the area shows the highest amount of pollutants.

Figure 3 shows the 1, 3-Butadiene zoning. According to the results, the highest concentration of the pollutant was 2141 ppb.

In Figure 4, the highest concentration of the pollutant in the northeast of the area was measured at 2164 ppb.

In summer, the highest concentration of 1, 3-Butadiene was measured at the north side of the area near Azadi Square. Also, higher levels of pollutants were measured in the west, northwest, and southeast sides of the area in comparison with spring.

Risk assessment

In carcinogenic and non-carcinogenic risk assessment, converting the ppm and ppb units to $\mu g/L$ or mg/L is required. Table 3 shows the 1, 3-Butadiene concentration risk in $\mu g/m^3$ for related calculations.

Table 4 was used to discuss cancerous risk assessment for different groups. First group included residents who lived in the area during the day, second people who traveled 2 h/day, this group was divided into two groups: pedestrians who traveled to and from

Table 1. Average measurement of 1, 3 Butadiene in seasons in different stations of District 9 of Tehran in 2019-2020

Sampling Point	3,1-Butadiene (ppb)				
	Autumn 2019	Winter 2020	Spring 2020	Summer 2020	
1	1006	982	891	916	
2	806	768	761	790	
3	647	645	615	534	
4	660	630	603	687	
5	474	664	458	442	
6	563	506	498	477	
7	488	466	446	477	
8	627	570	521	517	
9	470	455	424	439	
10	552	534	518	498	
11	558	489	472	454	
12	627	590	573	554	
13	593	571	552	654	
14	1065	930	813	1057	
15	1576	1376	1120	1456	
16	1481	1288	1032	1342	
17	2287	2027	1480	1850	
18	1327	1160	1015	1320	
19	1604	1400	1134	1174	
20	660	571	543	431	
21	722	626	543	706	
22	1205	1045	907	1179	
23	541	301	265	345	
24	1087	947	824	1081	
25	626	597	577	528	
26	785	684	596	775	
27	1478	2105	1451	1159	
28	1452	1375	911	981	
29	1113	970	845	1099	
30	2891	2141	2164	1245	

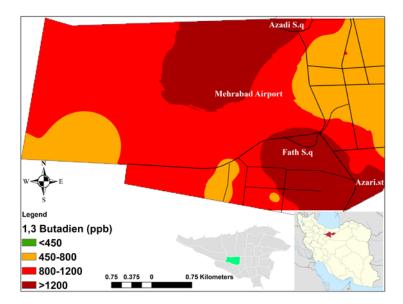


Figure 2. Zoning of 1, 3-Butadiene in autumn in the District 9 of Tehran

work and pedestrians who traveled to shop or did business. The last group was related to employees whose place of work was in District 9 of Tehran.

Table 5 lists the results of Chronic Daily Inhalation (CDI) 1, 3-Butadiene for different at-risk groups in District 9 of Tehran.

According to the CDI values for cancerous risks for different exposed groups, who are mentioned in this research, it is observed that the residents of the district had higher values for both cancerous risks than the other groups. Also, the class 2 pedestrians who had a lower time of presence in the area had the lowest amount of risk.

Table 6 lists the risk of cancer in the presence of 1, 3-Butadiene in different high-risk groups in District 9 of Tehran. These results were calculated on the basis of CDI for each group and in the seasons.

The carcinogenic and non-carcinogenic risk in different seasons was calculated for exposed groups in Table 6. The residents had the highest risks for both carcinogenic

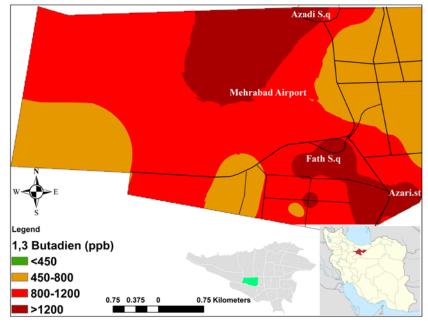


Figure 3. Zoning of 1, 3-Butadiene in winter in the District 9 of Tehran

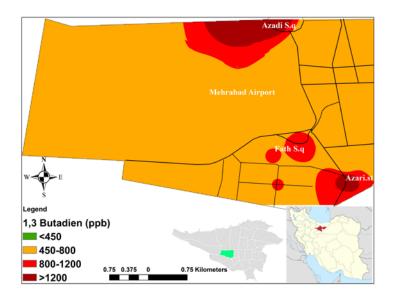


Figure 4. Zoning of 1, 3-Butadiene in spring in the District 9 of Tehran

and non-carcinogenic risk in autumn. This value in non-carcinogenic risk was higher than 1 for all the groups in all seasons except for the class one and two pedestrians.

4. Conclusion

1, 3-Butadiene is a known carcinogenic compound, but cancer risk assessments have not comprehensively been studied for many cities. The aim of this study was to evaluate the cancer risk of 1, 3-Butadiene release in District 9 of Tehran in autumn 2019 and winter, spring and summer 2020. The CDI estimates were examined in depth based on at-risk groups. Risk assessment showed

that all at-risk groups in the study had the LCR estimations exceeding the USEPA (United States Environmental Protection Agency) benchmark of 1×10^{-6} . According to the results, the risk of cancer was higher for the residents of the area. Given the traffic, this makes sense. Also, second-class pedestrians who traveled in the area 50 days a year had a lower risk than other groups. Also, the risk of cancer in all seasons was higher than the allowable limit (1×10^{-6}). The highest pollution occurred in autumn. The southwest side had the highest concentration of pollutants in this season, and in other seasons the north and northwest sides had the highest concentration. According to the heavy traffic of cars in autumn and cli-

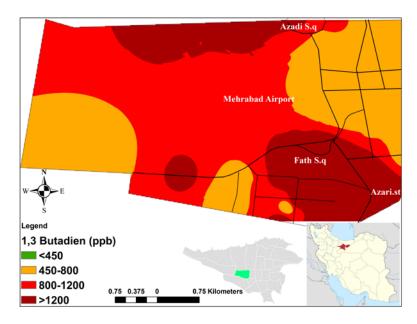


Figure 5. zoning of 1, 3-Butadiene in summer in the District 9 of Tehran

Table 2. Descriptive statistics and significant results of 1, 3-Butadiene in the seasons

Season	Mean±SD	Median	Mean Rank	df	χ²	Asymp. Sig.
Autumn	999.03±571.89	753.50	2.17			
Winter	913.77±500.41	674.00	1.4	2	F7 40	0.0001
Spring	785.07±395.05	609.00	2.57	3	57.48	0.0001
Summer	838.90±384.75	740.50	3.87			

Table 3. Conversion of mean concentrations of 1, 3-Butadiene from (ppb) to $(\mu g/m^3)$

Season	μg/m³	ppb
Autumn	452	999
Winter	413	914
Spring	355	785
Summer	379	839

Table 4. Risk determination groups in the exposure of 1, 3-Butadiene in District 9 of Tehran

Group	Exposure Rate	Number of Exposure Days	Exposure Dose
Residents	24	350	70 years
Passers-by 1	2	260	30 years
Passers-by 2	2	50	30 years
Staff	8	260	30 years

Table 5. Chronic Daily Inhalation (CDI) results of 1, 3-Butadiene in District 9 of Tehran

Group	Type of Risk	CDI
Residents	Cancerous risk	235×10 ⁻⁵
Passers-by 1	Cancerous risk	33.7×10⁻⁵
Passers-by 2	Cancerous risk	6.5×10 ⁻⁵
Staff	Cancerous risk	135.5×10⁻⁵

Table 6. Cancer risk of 1, 3-Butadiene release in Tehran's District 9 for four high-risk groups from autumn 2019 to summer 2020

Season	Residents	Passers-by 1	Passers-by 2	Staff
Autumn	790×10 ⁻⁶	22×10 ⁻⁶	120×10 ⁻⁶	460×10 ⁻⁶
Winter	730×10 ⁻⁶	20×10 ⁻⁶	110×10 ⁻⁶	420×10 ⁻⁶
Spring	630×10 ⁻⁶	10×10 ⁻⁶	90×10 ⁻⁶	360×10 ⁻⁶
Summer	670×10 ⁻⁶	19×10 ⁻⁶	96×10 ⁻⁶	390×10 ⁻⁶

mate parameters such as wind speed, wind direction, and temperature, these results made sense. Also, the highest carcinogenic and non-carcinogenic risks in autumn were for the residents' group and after them for the employees' group, showing that amount of exposure is a crucial factor in increasing this pollutant risk. At last, it seems that the cars traffic directly affects the level of 1, 3-Butadiene emission in the big cities' atmosphere. However, we cannot ignore the importance of the fuel quality of cars which can be a topic for other researchers to investigate and discuss. Also, in the study of pollutant emissions in the region, the amount of pollutants in the southwest, center, north and southeast of District 9 of Tehran in autumn, north and center of District 9th of Tehran in winter and the same areas in summer and a small part of the north in spring. They had 1, 3-Butadiene.

In general, the results showed that the amount of pollution was high in different areas of the region with high traffic streets. This pollution can endanger the health of the people living in this district. The risks due to the presence of the pollutants such as volatile organic compounds in cities were always in the spotlight for residents of that area because of their carcinogenicity properties. In this research, one of Tehran's high traffic and strategic area (the capital city of Iran) was selected to measure the 1, 3-Butadiene concentration.

There were limitations in the process of conducting this research. Including rainfall that delayed measurement. Also, switching between measuring points may be delayed due to traffic and may continue for hours of the night. Finally, in line with the research results, it is suggested that the effective parameters on the release of 1, 3-Butadiene should be known and a study should be performed. Improving the quality of production vehicles in terms of pollution, using alternative fuels and green fuels and studying how to break the bonds of volatile organic compounds, including 1, 3-Butadiene, are other research suggestions.

Ethical Considerations

Compliance with ethical guidelines

There were no ethical considerations to be considered in this research.

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Authors' contributions

All authors participated equally in the collection and analysis of data.

Conflict of interest

The authors declared no conflict of interest.

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