International Journal of Recent Technology and Engineering (IJRTE)
ISSN: 2277-3878 (Online), Volume-9 Issue-1, May 2020

Multivariate Statistical Analysis of Atmospheric Dispersion of BTX Compounds at Sanathnagar, Hyderabad.

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***Abstract:** Sanathnagar, located in the centre of Hyderabad city, is taken as a case study to assess the meteorological factors influencing the air quality parameters Benzene, Toluene, Xylene (BTX compounds) and to identify the significant sources of pollution using the interspecies ratios. A data of ten years (2007-2017) from Central Pollution control board (CPCB), Hyderabad, Telangana state is studied. TX compounds coming under Volatile Organic Compounds (VOC) were considered as the air quality parameters, seasons as cases and concerning meteorological factors such as Atmospheric Temperature AT (^{0}C), Relative Humidity RH(%), Wind Speed WS (m/s), Wind Direction WD (deg), Sun Radiation SR (w/m^{2}), Barometric Pressure BP (mm/Hg). Multivariate statistical techniques, namely Principal Component Analysis (PCA), and Cluster Analysis are used in this study with the help of IBM SPSS 26. The KMO test sampling adequacy found to be higher than 0.5, and the Bartlett test showed lesser value than 0.00, hence proving the results of the analysis are satisfactory. From BTX ratios it was observed that T/B was much higher than one and X/B been minimal value for all seasons indicating traffic pollution as a significant source of ambient air pollution in the study area.*

On the other hand, the correlation matrix states that a positive correlation between meteorological factors and ambient air quality parameters are as follows: SR- Benzene, Xylene; BP-Toluene; WS- Benzene, Toluene, and Xylene and the factors with a negative correlation on parameters are WD, RH, AT. PCA states that ambient air quality parameters are influenced by meteorological factors such as SR, RH, WS, WD (major influencers) and BP, AT (moderator influencers). Whereas in Cluster Analysis major influencers are WS, AT, RH and moderate are WP, SR, BP respectively. Therefore, PCA and CA results have shown similar trends in the categorization of meteorological influencers.

***Key words:** Principal Component Analysis, Factor Analysis, BTX Compounds, VOC Compounds, Interspecies ratios, Sanathnagar, Hyderabad.*

I. INTRODUCTION

Over some time, many scientific studies have proven the harmful impacts of Volatile Organic Compounds (VOC) in urban ambient air.

Manuscript received on April 02, 2020.
Revised Manuscript received on April 15, 2020.
Manuscript published on May 30, 2020.
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They are many studies related to respiratory diseases and cancer on the nearby inhabitants due to pollution from both industrial and traffic emissions [1]. Due to their toxicity BTX compounds are well correlated with each other and can be found in indoor, outdoor environments [2].

The concentration level of these compounds can vary between the seasons, year to year due to such reasons as source emissions, climatic conditions in the city, & the geographic location. A study stated that BTX concentrations are higher in winter than in summer due to chemical reaction rates of BTX with the dust storm that eventually removes the compounds in summer [3]. Meteorological parameters such as atmospheric turbulence and wind direction are to be responsible for daily modulation of BTX compounds [4].

As the ratios of B/T and T/B are essential to identify the emission sources in the study where vehicular emission act as a prominent mobile source as indicated by ratios of B/T, X/E reported by [5]. In another study the characterized Benzene, Toluene, Ethylbenzene, O & (m+p)-xylene concentrations and their relationships between two cities were studied to use interspecies ratio in identifying photochemical ageing and potential source origination of nearby sources [6].The BTX ratios are useful in recognizing the relationship between the pollutants and covariance, as well as dispersion, reaction pattern occurring during their transport across the cities [4].

The influence of seasonal variation on BTX hydrocarbons was given by stating Toluene is the most abundant VOC measured among other compound and has a maximum mean concentration in the winter season, lowest during summer [4] . At the same time, T/B (>1) ratio observed to indicate vehicular emission as the primary source.

Through most of the literature available on VOC compounds reported by scientific papers, studies on their correlation to seasonal variation using multivariate analysis are very limited. The aims of present work in the paper is to infer the variations in ambient air concentrations of BTX compounds in sanathnagar, Hyderabad on a seasonal basis and to study their interspecies ratio.

II. METHODOLOGY

A. Study area and data collection: The hourly atmospheric concentrations of BTX (Benzene, Toluene, and Xylene) are provided by CPCB (central pollution control board) for one sampling station "Sanathnagar" ($17^{0}29^{I}$N, $78^{0}25^{I}$E) in Hyderabad, Telangana state through the period of 2007-2017.CPCB uses Continuous Ambient air quality monitoring system (CAAQMS) to collect the ambient air quality data in 24 hourly formats, daily basis throughout the year.

Hyderabad witness four distinct seasons- summer, monsoon, post-monsoon and winter. Where summer season extends from March to June, monsoon season as July to September, Post monsoon from October-November and winter from December to February.

In this paper, seasons are taken as cases to study the relationship between meteorological data and ambient air quality parameters.

B. Statistical Analysis: Using IBM SPSS 26 software study of multivariate analysis is conducted, which comprises of the following methodology 1) Missing value data and validation of data 2) Principal Component Analysis 3) Cluster Analysis.

C. Missing value data and validation of data: As the collected data comprised of missing data more than 5%, which implies they cannot be ignored or else it might reduce the sample size. By applying the MCAR test to the data with missing values as an input, the P-Value is higher than 0.05, where multiple imputation method is to be best fitting one to replace the missing values. Validation of data is helpful to identify any invalid cases and data variable in a data set. The data obtained from the analysis of the missing values are given as an input for validation where the duplicate cases are identified and analysed by conducting the required statistical test.

D. Principal Component Analysis (PCA): Is conducted to detect the factors influencing the air quality parameters in each cluster produced by cluster analysis. In this process, new variables are formed from the existing set of variables.

E. Cluster Analysis: It is a statistical approach for sorting cases, observations or variables. For a set of data Hierarchical Agglomerative Cluster Analysis (HACA) is the commonly used technique to analyse the data. The output of the analysis a Dendogram is executed and examined from left to right. This output is used to identify a set of a meaningful subgroup.

III. RESULTS AND DISCUSSIONS

A. Seasonal variability of BTX Compounds in sanathnagar, Hyderabad: The seasonal mean concentration of monitored station shown in Table no:1 for the study period of 2007-2017. Benzene, Toluene, Xylene are the three Major volatile organic compounds considered in this study. All the yearly data are found to exhibit seasonal variability. Among BTX, Toluene was found to be the most abundant VOC in the Atmospheric concentrations of sanathnagar, Hyderabad. Similar trends observed by researchers in other urban areas such as [7] Neetu Bauri et al. 2015 in Deharadun, [6] Linsay Miller et al. 2011 in Canada, [5] Al-Harbi.M et al. 2018 in Kuwait, [4] C.Gariazo 2005 in Rome, [8] M.A Parra et al. 2008 in Spain.

Sanathnagar, Hyderabad being a residential cum industrial area located in the city centre. The activities here are concerned with Traffic-related pollution. Sanathnagar experienced a sequence of mean concentrations of BTX compound through the seasons in the study period as follows- Winter> Post-monsoon> Summer> Monsoon. The maximum mean of BTX compounds is observed in winters and minimum during summers. Toluene ambient concentration found to register highest during winter and lowest during monsoon season. In monsoon seasons Benzene and Xylene are observed to be comparatively lower than other seasons. BTX concentrations tend to get diluted because of heavy rains in the monsoon season [7]. It can be further supported as in the study area average monthly relative humidity was around to be 60.3% during monsoon season. Similar to BTX Trends in India for seasonal variations as observed are carried out by many researchers in different parts of the world. The mean ambient concentration of Benzene in all seasons is mostly exceeding standard limit 5µg/m3 set by CPCB. Benzene believed to be coming from emissions of cars is a carcinogenic volatile organic compound and responsible for having a direct link to respiratory diseases [9].

B. Interspecies ratios of BTX in Sanathnagar, Hyderabad: These ratios of T/B and X/B are used to indicate and identify emission sources. The mean interspecies ratio among BTX compounds is provided in Table no: 1 Traffic-related emission indicated by T/B (Toluene to Benzene) ratios. Benzene and Toluene are constituents of gasoline and mostly released into the atmosphere by motor vehicle exhaust. If T/B is higher than one, it indicates a significant source in Vehicular emission. From Table no: 1 highest T/B ratio was observed in post-monsoon for the years 2007 (7.73), 2008 (4.44), 2011 (11.07), 20.12 (7.69), 2016 (11.24), 2017 (19.83) than other seasons. Similarly, the X/B ratio observed to be maximum in winter season for the years 2007 (0.761), 2012 (1.88), 2015 (1.58) and in monsoon season for the year 2017 (1.97), Post-monsoon 2011(1.68)

Table no 1 : T/B and X/B ratios with respect to seasons

Season	Year	Benzene μgm^3	Toluene μgm^3	Xyelene μgm^3	T/B ratio	X/B ratio
Summer season	2007	5.02	17.55	2.16	3.50	0.43
	2008	4.68	14.08	3.13	3.01	0.67
	2009	6.49	37.17	6.74	5.73	1.04
	2010	4.60	38.11	9.35	8.29	2.03
	2011	1.69	10.19	2.12	6.02	1.25
	2012	1.07	6.06	0.67	5.64	0.62
	2015	1.29	14.00	2.72	10.83	2.10
	2016	0.86	7.89	0.97	9.14	1.13
	2017	0.31	4.38	0.47	13.99	1.52
Monsoon season	2007	3.69	7.44	1.29	2.01	0.35
	2008	3.59	5.59	0.83	1.56	0.23
	2009	3.60	19.85	3.95	5.52	1.10
	2010	2.88	14.99	3.58	5.20	1.24
	2011	0.43	2.43	0.54	5.59	1.24
	2012	5.13	16.81	4.24	3.28	0.83

	2015	2.11	10.30	0.34	4.87	0.16
	2016	0.51	4.34	0.49	8.53	0.96
	2017	0.65	9.96	1.30	15.22	**1.98**
Post-Monsoon season	2007	5.13	39.69	3.37	**7.74**	0.66
	2008	4.26	18.90	2.66	**4.44**	0.63
	2009	29.67	143.68	26.95	4.84	0.91
	2010	6.16	41.28	8.52	6.70	1.38
	2011	1.31	14.53	2.22	**11.07**	**1.69**
	2012	6.83	52.53	11.91	**7.69**	1.74
	2015	3.14	25.15	0.26	8.01	0.08
	2016	0.87	9.82	0.82	**11.25**	0.94
	2017	1.84	36.46	2.25	**19.83**	1.22
Winter season	2007	7.34	30.47	5.59	4.15	**0.76**
	2008	5.09	19.13	2.85	3.76	0.56
	2009	8.71	53.57	9.32	6.15	1.07
	2010	7.48	66.88	12.77	8.94	1.71
	2011	3.95	27.10	5.02	6.86	1.27
	2012	2.45	18.78	4.62	7.66	**1.88**
	2015	2.68	30.06	4.25	11.20	**1.58**
	2016	1.38	14.44	0.90	10.44	0.65
	2017	1.55	20.27	1.49	13.12	0.97

BTX concentrations showed higher on records during rush hours of morning and evening, implying a high volume of traffic. T/B and X/B ratios proposed vehicular emissions to be a predominant source for BTX concentrations. The interspecies ratios showed a seasonal variation, with higher concentrations of T/B ratios in post-monsoon and X/B ratios during the winter season.

C. Relationship between BTX compounds and Meteorological factors using Multivariate analysis.

In this paper, a study of the association between BTX compounds and meteorological factors was carried out. BTX & meteorological data as parameters, factors respectively and seasons as cases in the period 2007-2017 at sanathnagar, Hyderabad a correlation matrix is calculated using IBM SPSS 26. Table no: 2 shows maximum, minimum correlated parameters with meteorological factors, where the maximum values (positive sign) are considered as most influences factors on parameters and minimum values (negative sign) as minor influence factors.

The below table displays the strongest correlation between parameters and factors in four seasons as follows: In summer Benzene – SR, Toluene- SR, Xylene – SR, where as in monsoon Benzene – SR, Toluene – BP, Xylene - SR, where as in post-monsoon Benzene- SR, Toluene-SR, Xylene- SR and in winter season Benzene- SR, Toluene- SR, Xylene- SR. Therefore the correlation matrix states that a positive correlation between meteorological factors and ambient air quality parameters are as follows SR- Benzene, Xylene; BP- Toluene; WS- Benzene, Toluene, and xylene. And the factors with a negative correlation on parameters are WD, RH, AT.

Table No: 2 The major and minor influencing factors with correlation values, where positive sign stands for major influencer and negative stands for minor.

Parameters	Meteorological Factors					
Summer Season						
Parameters	AT (o C)	RH (%)	WS (m/s)	WD (deg)	SR (w/m2)	BP (mm/Hg)
Benzene (µg/m3)	-0.01	-0.68	0.12	-0.63	0.13	0.01
Toluene (µg/m3)	0	-0.84	0.13	-0.05	0.17	0.06
Xylene (µg/m3)	-0.05	-0.05	0.19	-0.07	0.22	0.14
Monsoon Season						
Parameters	AT (o C)	RH (%)	WS (m/s)	WD (deg)	SR (w/m2)	BP (mm/Hg)
Benzene (µg/m3)	-0.04	0.08	0.03	0.05	0.22	0.04
Toluene (µg/m3)	-0.06	0.03	-0.27	-0.02	0.03	0.05
Xylene (µg/m3)	-0.11	0.06	-0.18	-0.06	0.11	-0.14
Post-monsoon season						
Parameters	AT (o C)	RH (%)	WS (m/s)	WD (deg)	SR (w/m2)	BP (mm/Hg)
Benzene (µg/m3)	-0.07	-0.09	0.35	0.05	0.44	-0.25
Toluene (µg/m3)	-0.11	-0.16	0.01	-0.18	0.19	-0.4
Xylene (µg/m3)	-0.1	-0.1	0.02	0.01	0.22	-0.49
Winter Season						
Parameters	AT (o C)	RH (%)	WS (m/s)	WD (deg)	SR (w/m2)	BP (mm/Hg)
Benzene (µg/m3)	0.01	-0.09	0.22	-0.04	0.32	-0.16
Toluene (µg/m3)	0.04	-0.19	0.08	-0.06	0.26	-0.02
Xylene (µg/m3)	0.13	-2.11	0.1	-0.04	0.5	-0.41

D. Principal Component Analysis: Many researchers around the world concluded several Studies related to the correlation of meteorological factors and ambient air parameters. Where PCA (Principal Component Analysis) is used as a statistical tool to study the correlation, & used to find major and minor influencing factors. For example, a study of the ambient air of a city in the south-west of Mexico affected by the BTX levels and has a diurnal pattern showed highest concentrations in midday with as influence of wind direction [10] .

PCA is conducted to evaluate the clustering behaviour. Here the Eigenvalues greater than one are extracted and retained as components. Table no: 3 displays the retained and rotated components for PCA conducted for BTX compounds and six meteorological factors. The components higher than 0.75 are considered as strong, between 0.75-0.5 as moderate and less than 0.5 as weak influencers, respectively.

Table no:3 PCA of BTX compounds and meteorological parameters in the study period 2007-2017 considering seasons as cases

Cases	Components	Parameters
Summer season	PC1	Xylene (0.95), Toluene (0.92),Benzene (0.85)
	PC2	RH (0.79)
	PC3	WS (0.80)
	PC4	WD (0.82), AT (0.65)

Monsoon season	PC1	Xylene (0.94), Toluene (0.83),Benzene (0.84), RH (0.82)
	PC2	AT (0.86), SR (0.76), WD (0.89), BP (0.99)
	PC3	RH (0.83), WD (0.826), WS (0.59)
Post-Monsoon season	PC1	Toluene (0.95), Xylene (0.94), Benzene (0.82)
	PC2	AT (0.83)
	PC3	WS(0.77), SR (0.56)
Winter season	PC1	Xylene (0.90), Toluene (0.78), Benzene (0.688)
	PC2	AT (0.78) , BP (0.67)

Firstly a conclusion can be drawn that ambient air of the study area in sanathnagar, Hyderabad is effected by the BTX levels and also influenced by meteorological parameters. Secondly, Xylene, Toluene, Benzene are major gases pollutants and SR, RH, WS, WD been major and BP, AT as moderate influencers on the ambient air quality. As the Principal components (PCs) are changing season-wise only overall maximum values were taken into consideration.

Table no: 4 Eigen values, % variance and cumulative variance for BTX, Meteorological Compounds.

Cases	Components	Eigen values	% variance	Cumulative %
Summer	PC1	2.56	28.45	28.45
	PC2	1.39	15.40	43.85
	PC3	1.36	15.09	-
	PC4	1.19	13.18	-
Monsoon	PC1	2.42	26.87	26.87
	PC2	2.05	22.73	49.61
	PC3	1.69	18.76	**68.37**
Post-mosoon	PC1	2.64	29.31	29.31
	PC2	1.79	19.30	49.24
	PC3	1.70	18.86	**68.09**
Winter	PC1	2.55	28.34	28.34
	PC2	1.86	20.71	49.05

The % cumulative frequency is around 68.367 and 68.091 for monsoon, Post-monsoon seasons, respectively. The PC is PC3 in both the seasons, i.e. RH, WD, WS and SR can be named as major meteorological factors influencing the ambient air quality in the study area.

E. Cluster Analysis: In the summer season (fig no: 1**)** Two clusters are identified Cluster 1 (Benzene, Xylene, Toluene, WS, AT) named as highly correlated influencing factors. And Cluster 2 (WD, SR, BP) as moderately correlated influencing factors. The minimum distance between two stages is between Benzene – Xylene, Maximum distance between BP – WS. Total of eight stages and 9 Groups are formed. Whereas in the monsoon season (fig no: 2) two clusters, eight stages and nine groups are formed. In cluster 1 (Benzene, Toluene, Xylene, WS, AT, RH) and Cluster 2 (WD, SR, BP) have been noted. The maximum correlation is between Benzene- Xylene with the shortest distance, and the minimum correlation between BP- Xylene with maximum distance. Following monsoon season is Post-monsoon season (fig no 3) with an output of two clusters, eight groups, and nine cases. Cluster 1 (Benzene, Xylene, Toluene, WS, AT, RH) as major influencers and Cluster 2 (WD, SR, BP) as moderate influencers. Minimum distance (6604.68) with two highly correlated stages was between WS-Benzene, and the maximum distance is seen in among WS-BP with moderate correlation. And in the winter season (Fig no 4) two clusters, eight stages and 9 cases were formed. The highest influencing factors grouped as Cluster 1 (Benzene, Xylene, WS, Toluene, AT, RH) and moderately influencing factors are Cluster 2 (WD, SR, BP). The minimum distance was observed between Benzene and Xylene, whereas maximum distance is between SR and WD.

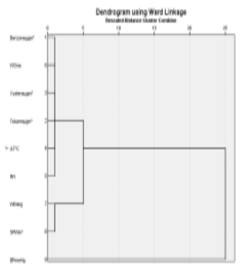

Fig no 1: Dendogram For Summer Season

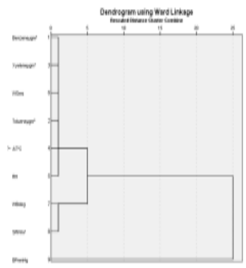

Fig no : 2 Dendogram for Monsoon

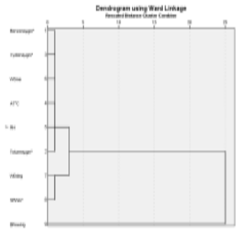

Fig no 3: Dendogram for Post-monsoon season

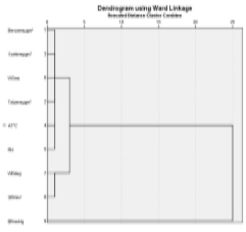

Fig no 4 Dendogram for Winter season

IV. CONCLUSIONS

1) Significant differences are noted while studying the BTX ratios in the study area regarding the variability for T/B and X/B ratio with respect to seasons and are as follows:

a) T/B ratio has shown a significant contribution of Benzene and Toluene compounds as area sources of traffic pollution in the study area.

b) Maximum and minimum ratios of X/B have been varied with the seasons, suggesting that the photochemical reactions are active. Smaller value of X/B ratio is an indication of vehicular pollution in the Sanathnagar, Hyderabad.

2) The relationship between BTX compounds and meteorological factors expose the following:

c) Correlation matrix states that a positive correlation between meteorological factors and ambient air quality parameters are as follows SR- Benzene, Xylene; BP- Toluene; WS- Benzene, Toluene, and Xylene. And the factors with a negative correlation on the pollutants are WD, RH, AT.

d) The ambient air of the study area that is Sanathnagar, Hyderabad is affected by the BTX levels and also influenced by meteorological parameters. The results from PCA state that Xylene, Toluene, Benzene are major gaseous pollutants and SR, RH, WS, WD been moderate and BP, AT as minor influencers on the ambient air quality.

e) Cluster Analysis results were varying according to season-wise. The major and minor influencing meteorological factors are WS, AT, RH and WD, SR, BP, respectively.

This paper suggests that ambient air quality monitoring and the relationship with meteorological factors shall be studied periodically concerning seasons, terrains, traffic volume to identify the dispersion of pollutants and alert the community of possible health risks.

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