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Comparative Analysis of Air Sampling Strategies for VOC Monitoring using TD-GCMS Along with Chemometrics Study to Enhance Understanding of Complex Samples

Praveen Arya[1], Anuraj Kumar[1], Abbey Fausett[2], Eric Fausett[2],Dr. Kiran Piduru[3]

[1]Agilent Technologies, Manesar, India

[2]Agilent Technologies, Littlefalls, DE

[3]Markes International, Bridgend, UK

Introduction

Monitoring volatile organic compounds (VOCs), is crucial for assessing air quality in industrial and urban environments. These compounds vary in volatility—from substances like propene to hexachlorobutadiene and naphthalene—and encompass both polar and non-polar chemicals. These pollutants, originating from industrial, vehicular, and urban sources, contribute to secondary aerosol formation and ground-level ozone, exacerbating air pollution.

- Sampling Methodologies: This study compares active and diffusive sampling techniques for VOCs in air.
- Active Sampling: Conducted at roadside, gas station, industrial, and residential sites using pumps to collect large air volumes, enhancing sensitivity for detecting low concentrations.
- Diffusive Sampling: Performed at industrial and residential areas without external equipment, suitable for remote locations and extended periods.
- Analysis: Samples were analyzed using Thermal Desorption-Gas Chromatography-Mass Spectrometry (TD-GC-MS), a solvent-free technique that preconcentrates analytes for automated injection into the GC-MS.
- Data Processing: Chemometric software tools, such as Mass Profiler Professional (MPP), were used for statistical analysis to process large datasets and identify patterns.

This study discusses the benefits of each sampling technique and their effectiveness in different locations, highlighting the importance of comprehensive air quality assessments.

Agilent 8890 & 5977C GCMS with Markes TD100-xr Thermal Desorber

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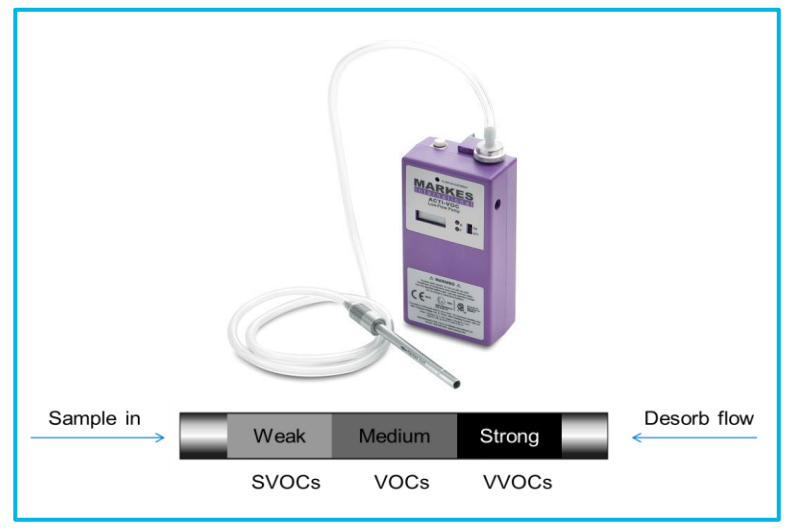
Experimental

Active Sampling Experiment:

Equipment: Clean, conditioned, and capped sorbent tubes (Markes' IS5182-28) with ACTI-VOC pump.

Procedure:

- Flow control at 20 ml/min for 1 hour.
- Tubes attached to pump, activated, and then capped post-sampling.
- Conducted at four locations: industrial, residential, traffic, and petrol station areas.



Active sampling of air through pump

Passive Sampling Experiment:

Equipment: Clean, conditioned, and capped sorbent tubes (Markes' IS5182-27) installed on Field Stations.

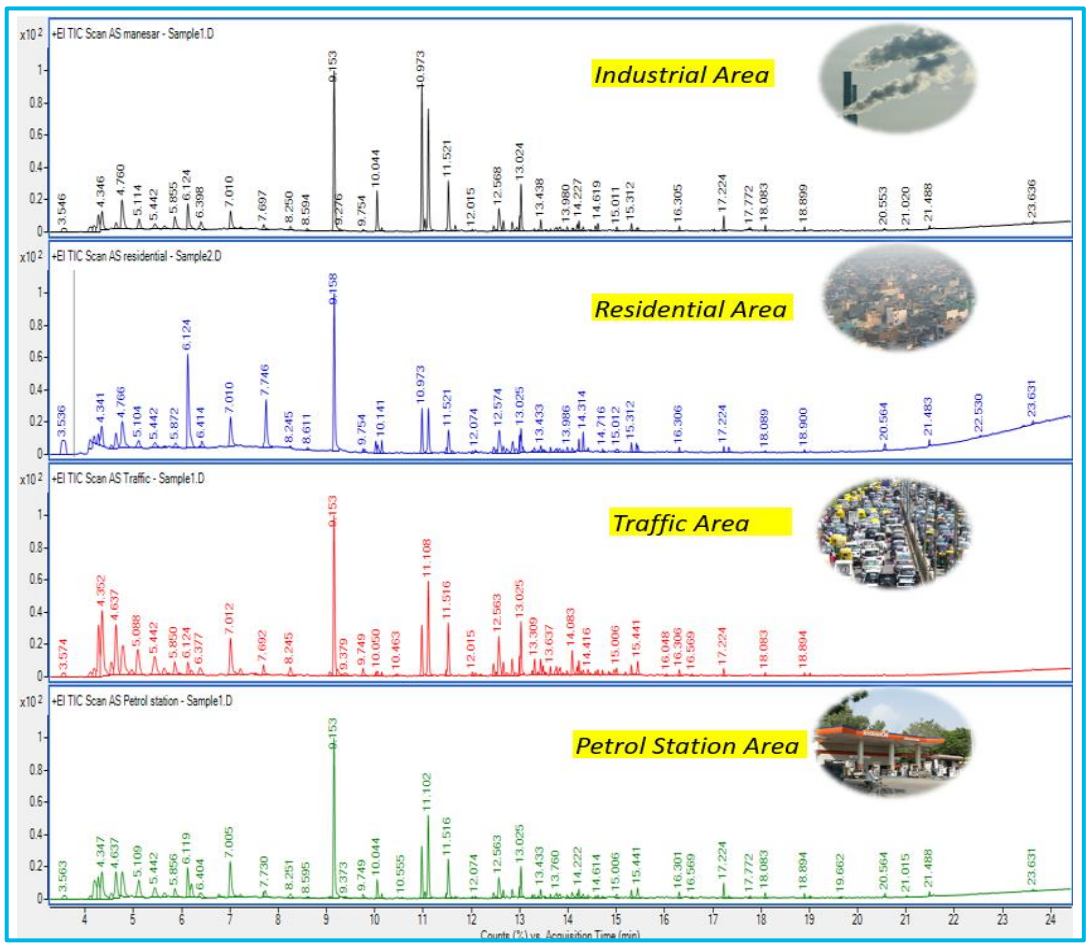
Procedure:

- Sampling in industrial and residential areas.
- Time periods: 24 hours, 1 week, and 2 weeks.
- Tubes capped post-sampling for lab transport.

Passive sampling of air in field station

Results and Discussion

Active Sampling Results:

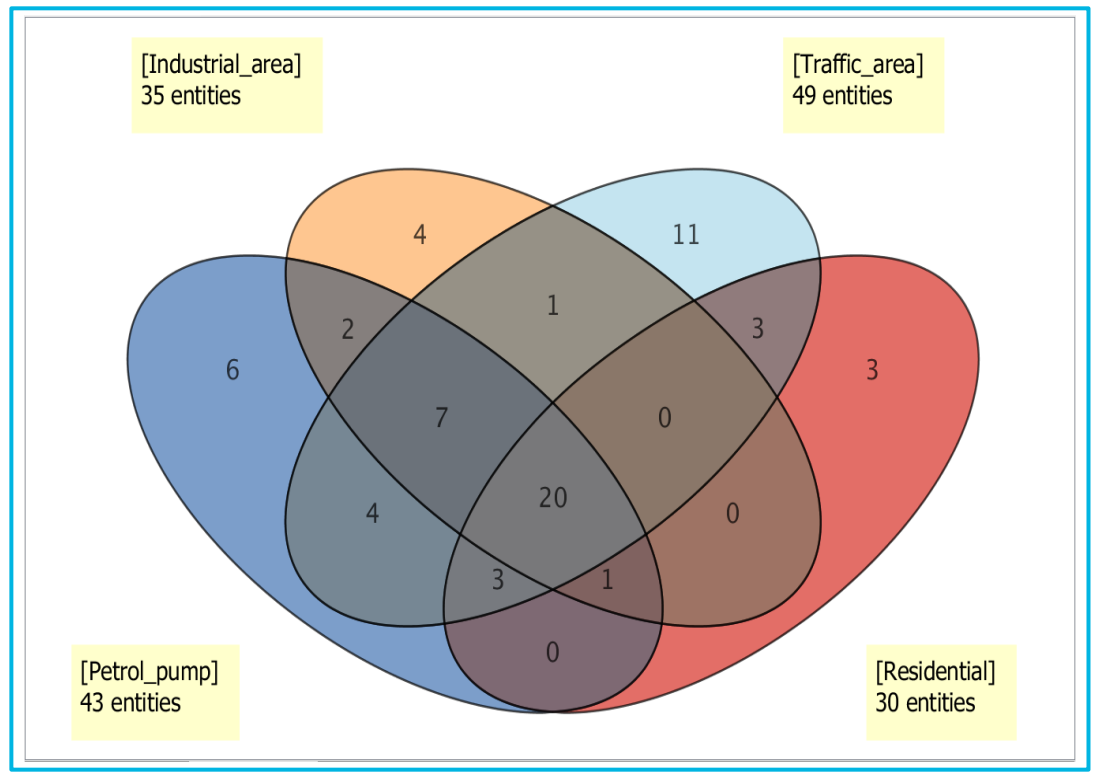


GCMS Chromatograms obtained for active sampling of air at various locations.

Hierarchical cluster analysis (HCA plot) showing the patterns of compounds obtained at various locations.

Active Sampling Results:

Chromatograms of air sampled at various locations shows presence of VOCs such as benzene, toluene, ethylbenzene and xylenes. Many common and unique compounds were found at each location. The intensity of these compounds shows variations at different locations. Fewer compounds with lower intensities were observed in air sample of residential area whereas, more compounds with higher intensities were observed in air sample of traffic area.



Venn diagram shows the number of unique and common compounds found in ambient air of each location

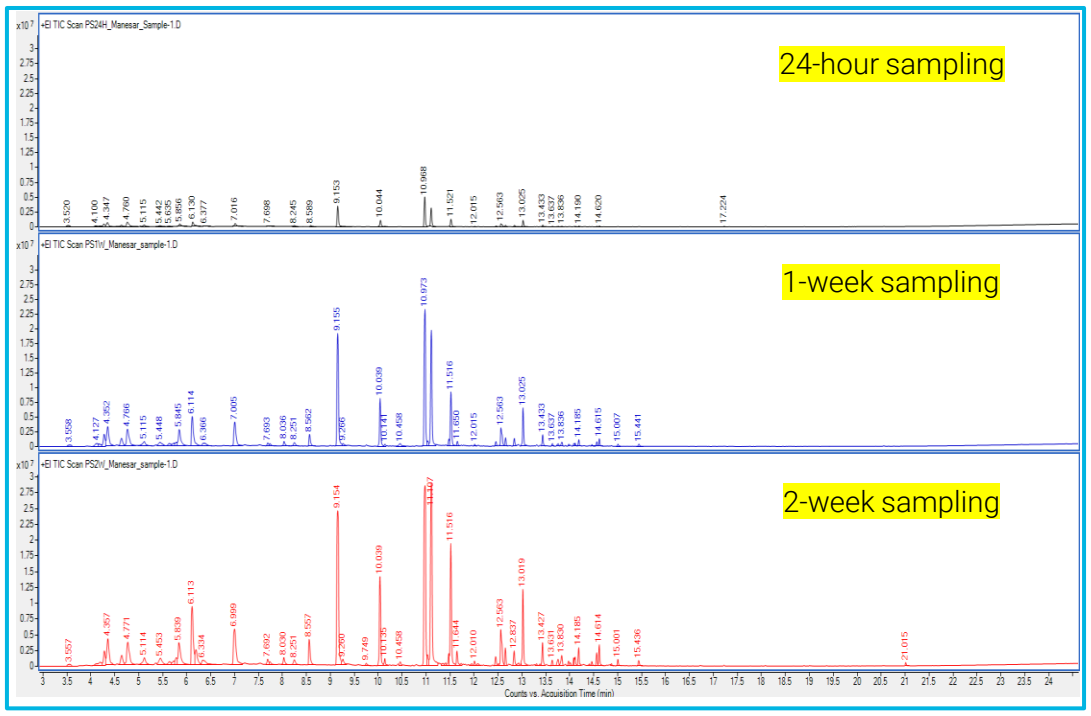
Unique compounds found at each location			
Industrial area	Petrol pump area	Traffic area	Residential area
Heptane, 2,2,4,6,6-pentamethyl-	Cyclohexane, 1,4-dimethyl-	Tricyclo[5.2.1.0(2,6)]dec-4-ene, 4-methyl-	Trichloroethylene
Hexadecane, 2,6,10,14-tetramethyl-	2-Naphthalenol, decahydro-	2-Heptene, (E)-	Cyclotetrasiloxane, octamethyl-
2-Ethoxyethyl acetate	2,4-Dimethyl-1-heptene	Heptane, 3-methyl-	Octanal
Tridecane, 6-methyl-	Propane, 1,2-dichloro-	3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene	
	Ethanol, 2-butoxy-	Linalool	
	Ethane, 1,2-dichloro-	Furan, 3-methyl-	
		Butane, 2,2-dimethyl-	
		Cyclohexane, 1,3-dimethyl-, cis-	
		Cyclohexanol, 5-methyl-2-(1-methylethyl)-	
		Cyclohexane, ethyl-	
		1H-Indene, 2,3-dihydro-1,6-dimethyl-	

Details of unique compounds found at each location

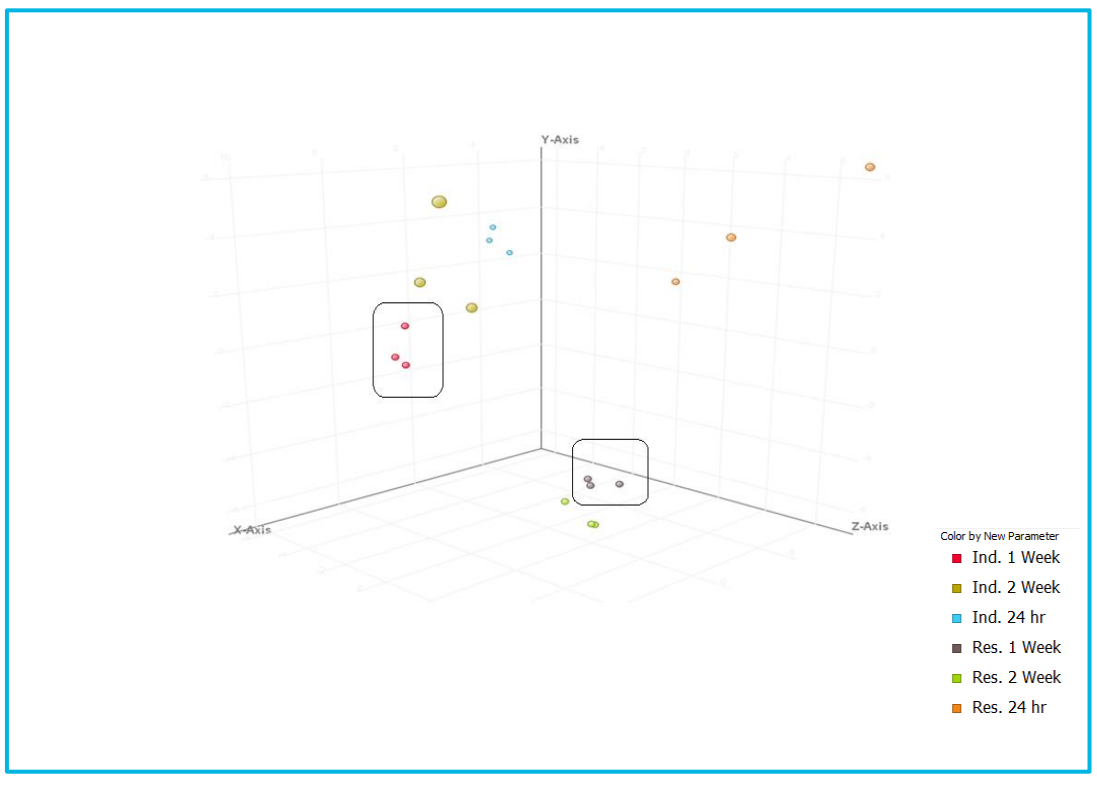
Results and Discussion

Passive Sampling Results:

The chromatographic overlays of different sampling time indicates an increasing trend in peak intensities with respect to time. There is considerable rise in peak intensities for 1 week sampling period as compared to 24-hour sampling. Whereas there is slight rise in peak intensities of 2-week sampling period as compared to 1-week sampling. The PCA plot suggest the peak distribution obtained in each data set. 1-week sampling results shows consistent replicate results.

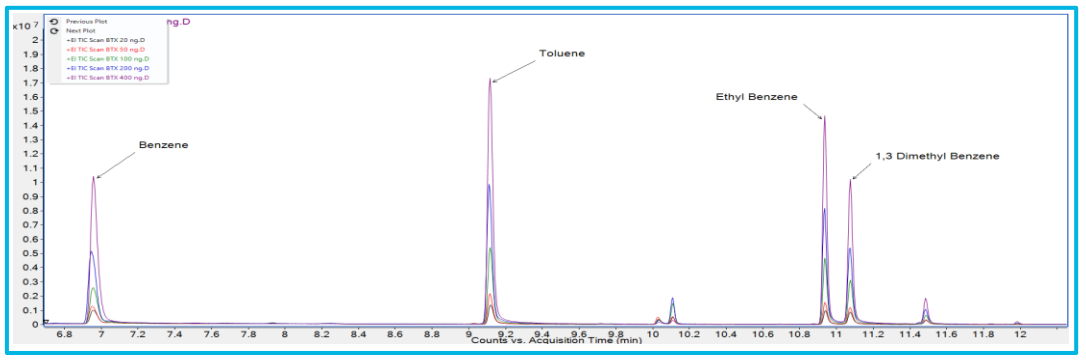


Chromatogram overlays for passive sampling at industrial area for sampling periods of 24 hrs, 1 week and 2 weeks respectively



PCA plot of passive sampling experiment to show the distribution among various samples

Quantitation of few VOCs (BTEX) in samples of both experiments:



Overlays for BTEX reference standards at 20 ng, 50 ng, 100 ng, 200 ng and 400 ng levels, respectively.

Active sampling BTEX quantitation				
Location	Benzene (ng/L)	Toluene (ng/L)	Ethyl Benzene (ng/L)	1,3-Dimethylbenzene (ng/L)
Industrial Area	3.9	174.9	191.1	234.8
Residential Area	1.4	39.5	9.7	16.4
Traffic Area	49.2	193.3	73.3	216.8
Petrol station Area	21.9	135.7	52.2	133.1

Passive sampling BTEX quantitation					
Location	Sampling time	Benzene (ng/L)	Toluene (ng/L)	Ethyl Benzene (ng/L)	1,3-Dimethylbenzene (ng/L)
Industrial area	24 Hour	9.8	82.4	175.1	158.7
	1 week	12.9	79.0	129.2	149.9
	2 week	6.8	58.1	90.0	127.5
Residential area	24 Hour	25.1	101.3	6.7	94.9
	1 week	19.7	72.0	37.1	53.5
	2 week	18.5	47.3	22.6	35.6

BTEX quantitation in samples

Conclusions

This study highlights the comparison of different air sampling strategies and shows their effect on qualitative and quantitative analysis of VOCs. Key highlights are:

- Active (pumped) sampling helps in faster analysis which is required for instant air monitoring.
- Passive sampling is comparatively a long-term approach and provides consistent results.
- Use of chemometrics software (MPP) has added value by data visualization for interpretation.

References

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