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Detection and Identification of Organic Compounds in Wastewater of Final Effluent Treatment Plant by FTIR and GC-MS

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ABSTRACT

The wastewater generated from multi-fold industrial estates is complex in nature because of the variability in the process system producing organic and inorganic load in the wastewater. These industries pollute water by discharging the wastewater containing large number of organics and other color causing compounds. Hence the area of interest is detection of wastewater components. Analytical methods such as FTIR and GC-MS have been used for the characterization of wastewater. The result achieved in the present investigation using GC-MS and FTIR study of sample confirms the presence of organics in wastewater. Efforts therefore have to be made provide some specific treatment employing advanced treatment methods/processes to improve the quality of wastewater to before discharging in the environment.

1. Introduction

Increasing urbanization and industrialization resulted in drastic increase in the volume of wastewater production around the world. Industries continuously release untreated effluents into rivers and other common sources of water; this industrial wastewater is the main source which pollutes water [1-3]. The wastewater generated from multi-fold industrial estates is complex in nature because of the variability in the process system producing organic and inorganic load in the wastewater. The scarcity of water resources around the world increases the demands on the use of secondary sources, such as wastewater. In this perspective water recycling and re-use of treated effluent in high water consuming industrial sectors seem be to be a viable alternative to save valuable resources [4, 5].

The generation of complex nature of wastewater and their treatment becomes very tedious because of the availability of multi-fold components and compounds, degradable and non-biodegradables and therefore represents a major environmental concern since most of the treatment systems being adopted or practiced are not feasible to remove such type of multi-nature components present in the wastewater. Now a days in case of water pollution high concentration of organics is most serious environmental problem [6]. In the last years, one of the major concerns to water quality is related to the detection of chemical pollutants in both industrial and municipal wastewater. Most of these contaminants, both synthetic organic chemicals and naturally occurring substances, enter the aquatic medium in several different ways and, according to their water solubility, can be transported and distributed in the water cycle [7]; of which color is the most visible pollutant that can be easily recognized in wastewater and it should be treated properly before discharging into water bodies or on land. The presence of color in wastewater either in industrial or domestics needs is considered as the most undesirable. Besides, the occurrence of various coloring agents like dyes, inorganics pigments, tannins and lignin which usually impart color [8] become among the main contributor for these environmental matter.

For the purpose of wastewater reuse and treatment it is important to characterize the compounds present in the industrial wastewater. In the present work, an attempt has been made to characterize the components

in effluent treatment plant using FTIR (Fourier Transform Infrared Spectroscopy) and GC-MS (Gas Chromatography-Mass Spectrometry).

2. Experimental Methods

Effluent water used in this study was obtained from the Final Effluent Treatment Plant of Ankleshwar, Gujarat, India. Final Effluent Treatment Plant (FETP), where industrial effluents from three industrial estates namely Ankleshwar, Panoli and Jhagadia are received and treated up to marine standards before conveying deep into the sea through a marine outfall. The characterization of wastewater has been carried out by FTIR and GC-MS spectrometer. Raw wastewater sample is shown in Fig. 1.



Fig. 1 Raw wastewater sample

For FTIR analysis the organic color compounds from the effluent are separated from waste water through complete evaporation. The potassium bromide (KBr, Fisher scientific IR grade) is oven dried to complete dryness and stored in desiccator until use. The compound–KBr mixture has been prepared by accurately weighing the KBr and organic compound. The mixture was quantitatively transferred to a mortar and ground with a pestle for 20-30 minutes to obtain a homogeneous mixture and a pellet has been prepared again. A pellet of same mass using pure KBr has been prepared similarly for blank reading. Analysis has been made for both the blank and organic compound KBr pellets using a FTIR-Perkinelmer, Spectrophotometer-400.

A sample was extracted with dichloromethane (CH_2Cl_2) [9-11] and organics extracted in organic layer were concentrated and sent GC-MS studies. The GC-MS instrument, Varian GC-450 and MS-240, USA, was used with the column DB-5, 30 m, 0.25 mm ID, 0.25 micron film thickness for

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the characterization of the various compounds in the wastewater sample. The GC-MS monitor depicting confirmation of identified compounds through inbuilt mass spectral library NIST 08, USA. The standard used for the GC-MS was of Dr. Ehrenstorfer. The analysis was carried under the following analytical conditions: temperature program, oven temperature, 60-270 °C with raise in 15 °C min⁻¹; and injection temperature, 270 °C; carrier gas, helium; flow rate, 1 mL/min; column, detector, mass spectrometer; mass range scanned, 50-1000 amu, respectively [12, 13].

3. Result and Discussion

3.1 FTIR Spectral Analysis

FT-IR spectroscopy, which is a complementary and extensively used method, gives information about the functional groups. The FTIR spectrum of raw wastewater sample is shown in Fig. 2. Below FTIR spectra functional groups detected are tabulated in Table 1.

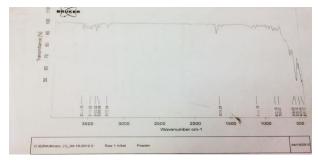


Fig. 2 FTIR Spectra of raw wastewater sample

Table 1 IR frequencies and detected functional groups from FTIR spectra

S. No. Wave number cm ⁻¹ Possibility of functional groups 1 3590.15 O-H stretch 2 3474.22 O-H stretch 3 3403.52 O-H stretch 4 3368.98 O-H stretch 5 3242.94 O-H stretch 6 1638.25 C=C stretch 7 1102.15 C-N stretch 8 836.28 R-Cl stretch 9 783.97 C-Cl stretch 10 558.00 C-Br stretch 11 538.12 C-Br stretch 12 490.54 C-I stretch 13 446.77 C-I stretch			
1 3590.15 O-H stretch 2 3474.22 O-H stretch 3 3403.52 O-H stretch 4 3368.98 O-H stretch 5 3242.94 O-H stretch 6 1638.25 C=C stretch 7 1102.15 C-N stretch 8 836.28 R-Cl stretch 9 783.97 C-Cl stretch 10 558.00 C-Br stretch 11 538.12 C-Br stretch 12 490.54 C-I stretch	S. No.	Wave number cm ⁻¹	Possibility of
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3 3403.52 O-H stretch 4 3368.98 O-H stretch 5 3242.94 O-H stretch 6 1638.25 C=C stretch 7 1102.15 C-N stretch 8 836.28 R-Cl stretch 9 783.97 C-Cl stretch 10 558.00 C-Br stretch 11 538.12 C-Br stretch 12 490.54 C-I stretch	1	3590.15	O-H stretch
4 3368.98 O-H stretch 5 3242.94 O-H stretch 6 1638.25 C=C stretch 7 1102.15 C-N stretch 8 836.28 R-Cl stretch 9 783.97 C-Cl stretch 10 558.00 C-Br stretch 11 538.12 C-Br stretch 12 490.54 C-I stretch	2	3474.22	O-H stretch
5 3242.94 O-H stretch 6 1638.25 C=C stretch 7 1102.15 C-N stretch 8 836.28 R-Cl stretch 9 783.97 C-Cl stretch 10 558.00 C-Br stretch 11 538.12 C-Br stretch 12 490.54 C-I stretch		3403.52	O-H stretch
6 1638.25 C=C stretch 7 1102.15 C-N stretch 8 836.28 R-Cl stretch 9 783.97 C-Cl stretch 10 558.00 C-Br stretch 11 538.12 C-Br stretch 12 490.54 C-I stretch		3368.98	O-H stretch
7 1102.15 C-N stretch 8 836.28 R-Cl stretch 9 783.97 C-Cl stretch 10 558.00 C-Br stretch 11 538.12 C-Br stretch 12 490.54 C-I stretch	5	3242.94	O-H stretch
8 836.28 R-Cl stretch 9 783.97 C-Cl stretch 10 558.00 C-Br stretch 11 538.12 C-Br stretch 12 490.54 C-I stretch	6	1638.25	C=C stretch
9 783.97 C-Cl stretch 10 558.00 C-Br stretch 11 538.12 C-Br stretch 12 490.54 C-I stretch	7	1102.15	C-N stretch
10 558.00 C-Br stretch 11 538.12 C-Br stretch 12 490.54 C-I stretch	8	836.28	R-Cl stretch
11 538.12 C-Br stretch 12 490.54 C-I stretch	9	783.97	C-Cl stretch
12 490.54 C-I stretch	10	558.00	C-Br stretch
	11	538.12	C-Br stretch
13 446.77 C-I stretch	12	490.54	C-I stretch
	13	446.77	C-I stretch

The absorption at 3590.15-3403.52 cm- 1 is attributed to O-H stretching corresponding to the alcohol and phenol groups in industrial wastewater, the absorption at 3368.98 cm- 1 resembles N-H stretching of primary amines, amides, and 3242.94 cm- 1 indicates to the O-H stretching of carboxylic groups. 1638.25 cm- 1 stretching resembles to the aromatic skeleton vibrations, while the band 1102.15 cm- 1 is attributed to C-N stretch; the stretch 836.28-783.97 cm- 1 indicates R-Cl groups; while 558.00-538.12 cm- 1 is attributed to C-Br stretch; 490.44-446.77 cm- 1 is attributed to C-I stretch. These spectra show the presence of some of the alcohol and phenol groups and having some amine and amine groups with aromatic skeleton.

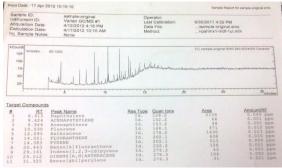


Fig. 3 GC-MS spectra of raw wastewater sample

3.2 GC-MS Analysis

The GC-MS technique is advanced and commonly used for determination of organic compounds in water samples [11, 14]. Also it is the combined application of gas chromatography and mass spectroscopy.

The gas chromatography separates different components in sample on the basis of their retention times resulting in peaks in gas chromatogram. The GC spectrum of raw wastewater sample is shown in Fig. 3. Organic compounds found in raw industrial wastewater are shown in Table 2.

Table 2 Organic compounds detected in GC-MS spectra of raw wastewater

Sr. No.	Name of Compound	Molecular Formula
1	Naphthalene	$C_{10}H_{8}$
2	Acenaphthylene	$C_{12}H_{8}$
3	Acenaphthene	$C_{12}H_{10}$
4	Fluorene	$C_{13}H_{10}$
5	Anthracene	$C_{14}H_{10}$
6	Fluoranthene	$C_{16}H_{10}$
7	Pyrene	$C_{16}H_{10}$
8	Benzo[k]fluroranthene	$C_{20}H_{12}$
9	Indeno[1,2,3-cd]Pyrene	$C_{22}H_{12}$
10	Dibenz[A,H]Anthracene	$C_{22}H_{14}$
11	Benzo[ghi]perylene	$C_{22}H_{12}$

The organic compounds found in effluent water were naphthalene, acenaphthylene, acenaphthene, fluorene, anthracene, fluoranthene, benzo[k]fluroranthene, indeno[1,2,3cd]pyrene, dibenz[a,h]anthracene, benzo[ghi]perylene.

4. Conclusion

The result achieved in the present investigation using GC-MS study of sample confirms the presence of organics in wastewater. Many forms of organic compounds in the form of PAH in wastewater are toxic to humans and aquatic environment. In FTIR analysis it is found the presence of alcohol, phenol sand amine groups may be responsible for the color of the wastewater due to the complex nature of the wastewater. The contamination of combined multi-complex compounds in wastewater becomes very toxic. Efforts therefore have to be made either to control the wastewater quality at the FETP inlet or provide some specific treatment employing advanced treatment methods/processes to improve the quality of treated wastewater.

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