Identification of Diesel Residues by GC-MS in Fire

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***Abstract*—In this paper, the application of Gas Chromatography-Mass Spectrometry (GC-MS) in diesel composition and its interference analysis was studied. The results show that the fresh diesel fuel sample mainly contains 13 kinds of aromatic compounds, and the characteristic compound group and component distribution can be clearly observed in diesel. The ion chromatography of polyurethane wood and diesel are basically the same, polyurethane wood has a great interference with diesel in fire identification. Therefore, it is feasible to analysis the distribution of diesel components using GC-MS technology.**

Keywords—diesel; GC-MS; compositions distribution; polyurethane wood

I. INTRODUCTION

Among the many fires that occur in the world every year, arson represents the worst cause. In the case of arson, fire accelerants, such as diesel, is often used to start fires. It is considered a serious crime to cause loss of life and property caused by arson[1-2]. Hence, high priority has been placed on arson investigation. Fire investigation must be carried out quickly in order to obtain the best chance for detecting diesel fuel residues in arson fire[3-4].

Diesel is one of the most highly refined products leaving the refinely. Diesel contains essentially all classes of hydrocarbons in the C_8-C_{23} range, but mainly aromatic compounds, with the alkylbenezenes being the most abundant and with a lesser abundance of naphthalene-based and indane-based compounds. Additionally, distributions and species of these compounds are different with materials[5-6].

In the present work a study was composition and interference to diesel by Gas Chromatography-Mass Spectrometry. GC-MS makes use of the high separation capacity of chromatography and the high identification characteristics of mass spectrometry, which can be used for the separation, qualitative and quantitative analysis of complex mixed samples. It is a perfect modern analytical method. At present, GC-MS has been well applied in the analysis of fire residues. In this paper, we apply GC-MS to the detection of diesel residues, commonly referred to as accelerants, and provide new data. It is able to accurately determine its composition and provide reliable technical support for the identification of physical evidence in arson cases[7-8].

II. EXPERIMENTAL SET-UP

The diesel used throughout the study was Ordinary 0# diesel purchased from a local gas station and the polyurethane wood purchased from a local store. All obtained samples were analyzed using an Agilent Technologies 7890B gas chromatograph. The following parameters were selected: Column: HP-5MS (30m×0.25 mm, 0.25μm film thickness); carrier gas: helium at 1 mL/min constant flow; inlet temperature: 250℃; split ratio:5:1; The GC oven temperature program used was: 40 ℃ isotherm for 2 min, increased by 5℃ min^{-1} to 80℃ and then increased by 10℃ min^{-1} to 280℃ (held for 5 min); mass spectrometer ionization source at 230 ℃; mass quadrupole analyzer at 150℃ in scan mode (m/z 50–550).

A. Extraction Preparation

For the study, Solid-phase microextraction (SPME) were used to extract diesel. The SPME fiber types used in this work were a 100μm PDMS which were obtained from Supelco, Bellefonte, PA, USA. PDMS fiber was inserted into the can for 50℃ and headspace for 30min, then retracted and inserted into the 250℃ injection port of HP 7890B chromatograph for 3min and analyzed.

III. RESULTS AND DISCUSSION

A. Compositions of Diesel Fuel

Figure 1 shows the total ion chromatogram of diesel. Diesel is usually composed mainly of aromatic compounds in the range C_{12} to C_{22}. All components of diesel were detected within 30 minutes and labeled under experimental conditions. The component pattern is a Gaussian distribution (bell-shaped curve), as shown in Figure 1.

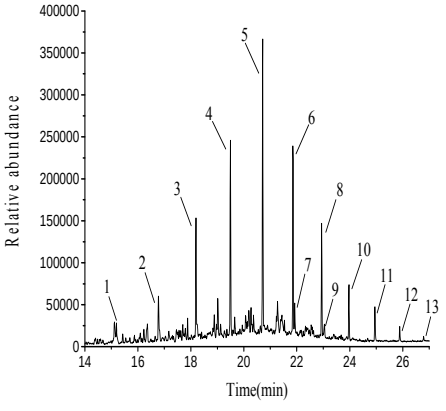

FIGURE I. TOTAL ION CHROMATOGRAM OF DIESEL

13 kinds of target compounds were detected by GC/MS as shown in Table 1. Pattern recognition was of great significance for the detection and characterization of diesel. All target

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compounds were confirmed by NIST database, SATURN database and related literatures. The results show that in the diesel containing not only dodecane, tridecane, tetradecane, pentadecane, hexadcane, heptadecane, octadecane, nonadecane, eicosane, heneicosane, docosane etc, but also have pristane and phytane. The use of GC-MS allows direct comparison of standard compounds with combustion materials to determine the type of accelerator used in a fire. Due to the high selectivity of GC-MS, since the matrix compound of the sample can be eliminated, so that an excellent correlation can be obtained. GC-MS is able to accurately determine its composition and provide reliable technical support for the identification of physical evidence in arson cases.

TABLE I. ID FILE FOR DIESEL TARGET COMPOUNDS

NO	*Target compounds*	*Retention time (min)*	*Formula*
1	Dodecane	15.197	$C_{12}H_{26}$
2	Tridecane	16.782	$C_{13}H_{28}$
3	Tetradecane	18.197	$C_{14}H_{30}$
4	Pentadecane	19.499	$C_{15}H_{23}$
5	Hexadecane	20.721	$C_{16}H_{34}$
6	Heptadecane	21.834	$C_{17}H_{36}$
7	Pristane	21.923	$C_{19}H_{40}$
8	Octadecane	22.955	$C_{18}H_{38}$
9	Phytane	23.044	$C_{20}H_{42}$
10	Nonadecane	23.962	$C_{19}H_{40}$
11	Eicosane	24.953	$C_{20}H_{42}$
12	Heneicosane	25.895	$C_{21}H_{44}$
13	Docosane	26.789	$C_{22}H_{46}$

IV. INTERFERENCE OF POLYURETHANE WOOD ON DIESEL

A total of compounds were detected in the diesel and polyurethane wood by GC-MS. For ease of observation and comparison of the interference of polyurethane wood on diesel, there are extracted ion chromatogram of 4 kinds of mass-to-charge ratios.

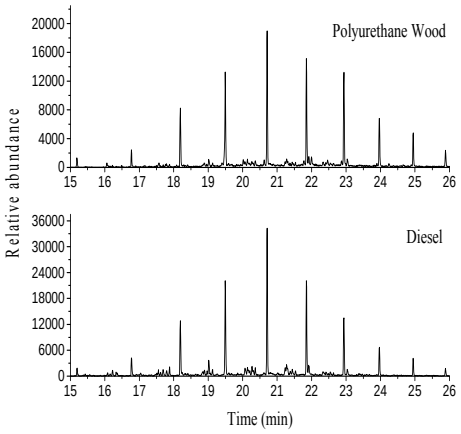

FIGURE II. COMPARISON OF POLYURETHANE WOOD WITH DIESEL (M/Z =85)

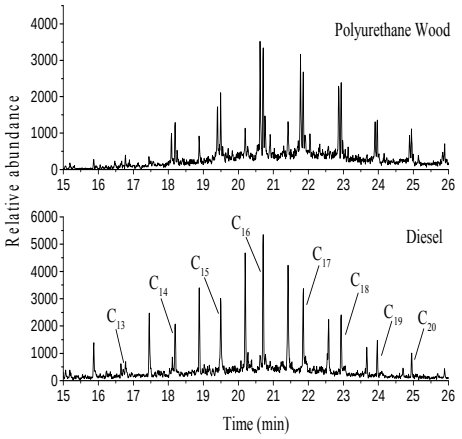

FIGURE III. COMPARISON OF POLYURETHANE WOOD WITH DIESEL（M/Z =83）

Figure 2 shows the ion chromatogram of compounds (m/z=85) extracted from polyurethane wood and diesel. As can be seen from the figure 2 that the ion chromatography of them is basically the same, polyurethane wood has a great interference with diesel. The pattern of the components is a gaussian (bell-shaped curve) .

Figure 3 shows the ion chromatogram of compounds (m/z=83) extracted from polyurethane wood and diesel, As can be seen from the figure 3 that diesel contains 8 compounds not found in polyurethane wood, it has relatively little interference with diesel.

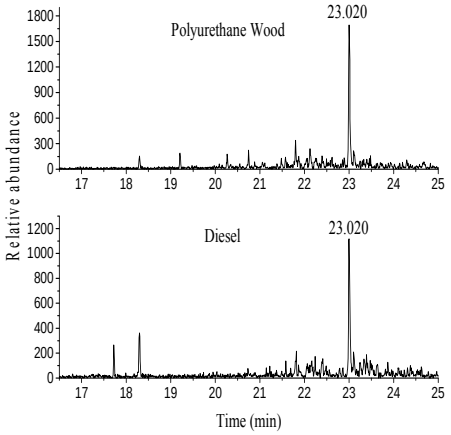

FIGURE IV. COMPARISON OF POLYURETHANE WOOD WITH DIESEL (M/Z =178)

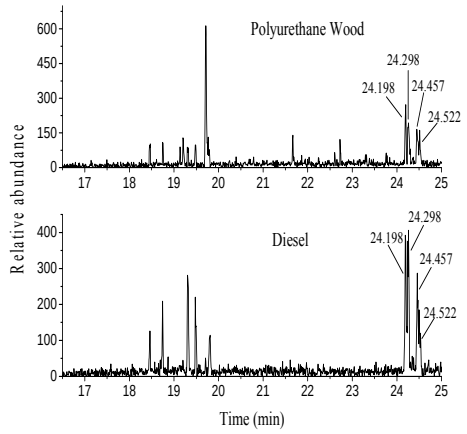

FIGURE V. COMPARISON OF POLYURETHANE WOOD WITH DIESEL (M/Z =192)

Figure 4 shows the ion chromatogram of compounds (m/z=178) extracted from polyurethane wood and diesel. As can be seen from the figure 4 that the ion chromatography of them is basically the same, their retention time was 23.020 min, it has a great interference with diesel in fire identification.

Figure 5 shows the ion chromatogram of compounds (m/z=192) extracted from polyurethane wood and diesel. As can be seen from the figure 5 that the ion chromatography of them is basically the same. There are two double peaks in 24.198 min and 24.298 min, 24.457 min and 24.522 min.

V. CONCLUSIONS

13 kinds of compositions in diesel were analyzed by GC-MS. The distribution of the groups of the characteristic compounds and their compositions were obtained. The pattern of the components is a gaussian (bell-shaped curve). Pattern recognition was of great significance for the detection and characterization of diesel. We also analyzed the interference of polyurethane wood on diesel. The results from above research show that polyurethane wood has a great interference with diesel, the ion chromatography of them is basically the same. GC-MS is able to accurately determine its composition and provide reliable technical support for the identification of physical evidence in arson cases. In order to accurately identify fire debris, it is very important to obtain diesel composition distribution and database. Finally, the results of this study confirm and support the need to collect and analyze negative control samples of substrates present in fire scenes.

ACKNOWLEDGMENT

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