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Application News

GC-MS GCMS-QP2050

Analysis of SAF Using Comprehensive Two-Dimensional Gas Chromatography (GC× GC)

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User Benefits

- ◆ By comparing chromatograms obtained as two-dimensional images, it can be utilized for quality control Inspection of SAF.
- ◆ Changing the column combination customizes separation characteristics to the sample composition.
- ◆ Utilizing the FASST (Fast Automated Scan/SIM Type) allows for the simultaneous analysis of the composition of SAF and the quantitative analysis of antioxidants.

■ Introduction

SAF (Sustainable Aviation Fuel) produced from waste cooking oil, used paper, and sugarcane has gained attention in recent years from the perspective of achieving a carbon neutral society. The physical properties of SAF, such as combustibility, vary depending on its components. Therefore, component analysis of SAF is crucial; however, since SAF is a mixture of various hydrocarbons, complete separation of each component is extremely challenging. Comprehensive two-dimensional gas chromatography (GC×GC), which utilizes the separation characteristics of two different types of columns, is an effective method for analyzing SAF with such a complex composition. Additionally, the GCMS-QP2050 enables ultra-fast scanning (30,000 u/sec), which improves the separation of adjacent peaks and allows for high-precision qualitative analysis(Application News No.01-00788-EN).

In this application, two types of SAF (A and B) and one intermediate product from the SAF production process (C) were measured using a combination of GC×GC with a non-polar column as the first column and a medium-polarity column as the second column. The two-dimensional images allow for a visual representation of the composition distribution, making quality control Inspection. Moreover, high separation of paraffins and naphthenes using a combination of a medium-polar column as the first column and a non-polar column as the second column, as well as the quantification of antioxidants in SAF, which are regulated by concentration in ASTM D2425 will be introduced.

■ System Configuration

The system configuration is shown in Tables 1. In this analysis, the ZX1 modulator from Zoex Corp. (Houston, TX, USA) was used. This modulator features thermal modulation using liquid nitrogen, allowing for the attainment of sharp peaks, including those of low-boiling compounds.

Table 1 System Configuration

GC Model	: Nexis™ GC-2030 / AOC-30i
MS Model	: GCMS-QP2050 (TMP exhaust: 255 L/sec)
Injection Port	: SPL
Modulator	: ZX1 thermal modulator (ZOEX corp.)
Nitrogen generator	: MT-24F (System Instruments Co., Ltd.)
Software	: Labsolutions™ GCMS GC Image (GC Image, LLC)
Library	: NIST Mass Spectral Library

Table 2 Analysis Conditions of SAF (Low polarity →Medium polarity)

GC	
1st Column	: DB-5MS (30 m × 0.25 mm I.D., df= 0.25 µm)
2nd Column	: BPX-50 (P/N：054740) (2.5 m × 0.10 mm I.D., df= 0.10 µm) *cut the column into 2.5 m
Injection Temperature	: 280 ˚C
Flow Control Mode	: Pressure (He)
Inlet pressure Program	: 150 kPa → 0.6 kPa/min → 200 kPa → 1.2 kPa/min → 250 kPa
Purge Flow	: 3 mL/min
Injection Volume	: 0.2 µL
Split ratio	: 100
Column Oven Temp. Program	: 40 ˚C → 1.0 ˚C/min → 120 ˚C → 2.0 ˚C/min → 220 ˚C → 4.0 ˚C/min → 280 ˚C (15 min)
MS	
Ion Source Temperature	: 230 ˚C
Interface Temperature	: 280 ˚C
Measurement Mode	: Scan
Scan Range (*m/z*)	: 35-500
Event Time	: 0.02 s (= 50 Hz、 30,000 u/sec)
Modulator	
Modulation period	: 6 s
Hot pulse duration	: 350 ms (320 ˚C)
Cold Gas Flow	: 15 L/min (N_2)

■ Comparison of SAF 2D images (Low-polarity → Medium-polarity)

An analysis of three different samples (A, B, and C) were conducted. The analysis conditions are shown in Table 2, and the obtained two-dimensional images are presented in Figure 1. A low-polar column, DB-5MS, was used as the first column, and a medium-polar column, BPX-50, was used as the second column. In this combination of columns, the horizontal axis represents boiling point, while the vertical axis corresponds to polarity. Sample A contains fewer aromatic compounds and naphthenes compared to sample B. Sample C is composed solely of low-boiling paraffins and naphthenes. Thus, by comparing two-dimensional images, intuitive comprehension of compounds distribution can be achieved, making it applicable for quality control of SAF.

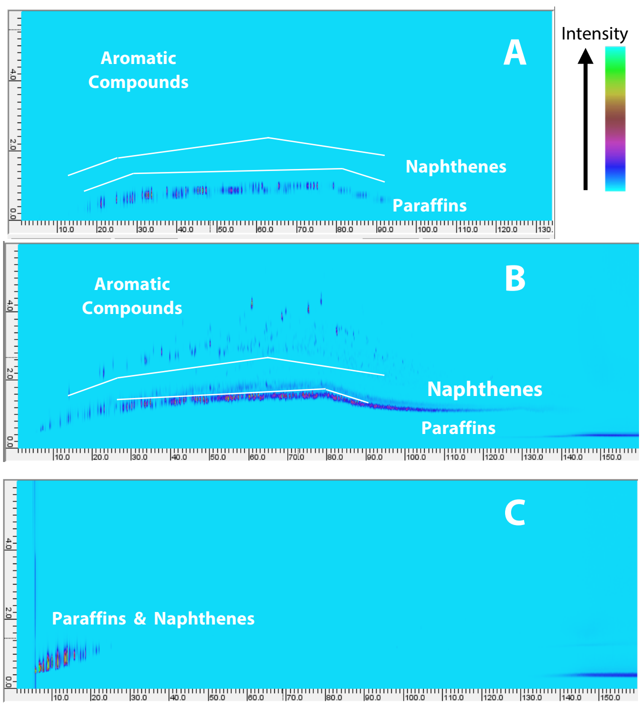

Fig. 1 TIC two-dimensional plot of the analysis of SAF samples (Low-polarity → Medium-polarity)

■ Medium-polarity → Non-polarity

In SAF that contains a high amount of paraffins and naphthenes, using a medium-polar column (SH-17) as the first column and a non-polar column (SH-1) as the second column is effective for improving their separation. In this case, the distribution differs from that of the previously mentioned combination of low-polar and medium-polar columns, with lower polar compounds being distributed towards the upper position. An example of a two-dimensional image is shown in Figure 2, where it can be seen that paraffins and naphthenes are separated over a wide range of retention times.

Additionally, clear separation was observed in the region of naphthenes and aromatic compounds. For paraffins, both straight-chain and branched types were separated vertically by the second column, making them easy to distinguish. Furthermore, the distribution of monoaromatic and diaromatic compounds was also distinguishable. In the analysis of diesel fuel, monocyclic, bicyclic, and tricyclic aromatic compounds can be distinguished from each other (Figure 3). The analysis conditions for SAF and diesel fuel are shown in Tables 3 and 4, respectively.

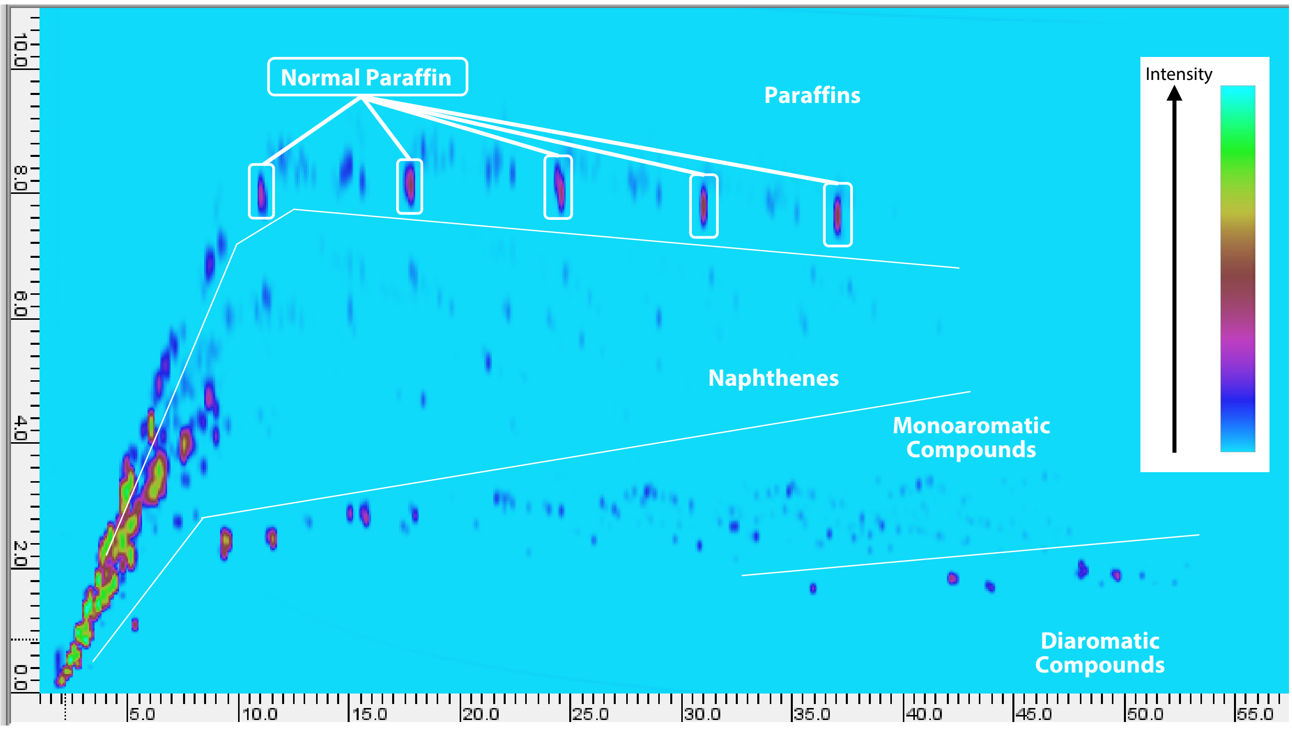

Fig. 2 TIC two-dimensional plot of the analysis of SAF sample (Medium-polarity → Non-polarity)

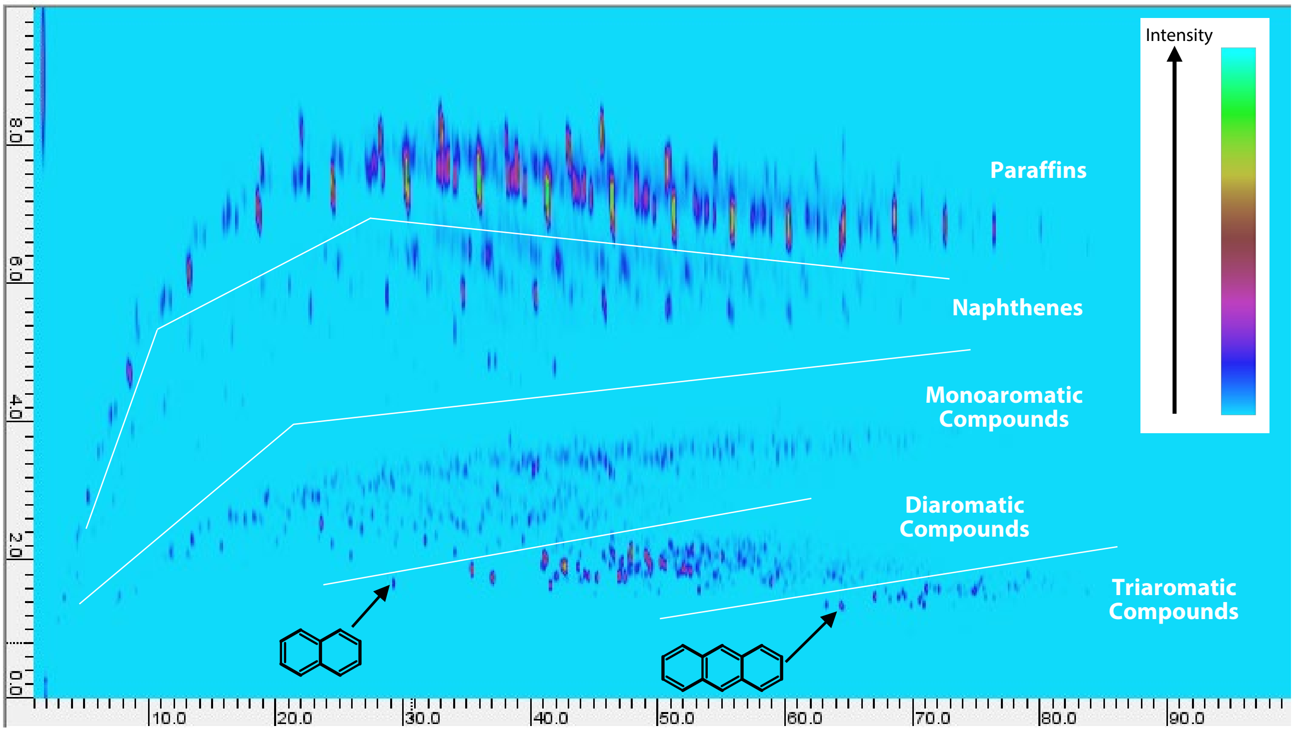

Fig. 3 TIC two-dimensional plot of the analysis of diesel sample (Medium-polarity → Non-polarity)

Table 3 Analysis Conditions of SAF (Low polarity→Medium polarity)

GC	
1st Column	: SH-17 (P/N : 221-75907-30) (30 m × 0.25 mm I.D., df= 0.25 µm)
2nd Column	: SH-1 (P/N : 221-75723-30) (2.5 m × 0.32 mm I.D., df= 0.25 µm) *cut the column into 2.5 m
Injection Temperature	: 250 ˚C
Flow Control Mode	: Pressure (He)
Inlet pressure Program	: 20 kPa → 1.0 kPa/min → 30 kPa → 2.0 kPa/min → 180 kPa
Purge Flow	: 3 mL/min
Injection Volume	: 0.1 µL
Split ratio	: 200
Column Oven Temp. Program	: 40 ˚C → 0.5 ˚C/min → 45 ˚C → 2.0 ˚C/min → 195 ˚C
MS	
Ion Source Temperature	: 230 ˚C
Interface Temperature	: 280 ˚C
Measurement Mode	: Scan
Scan Range (*m/z*)	: 35-500
Event Time	: 0.02 s (= 50 Hz、 30,000 u/sec)
Modulator	
Modulation period	: 11 s
Hot pulse duration	: 350 ms (350 ˚C)
Cold Gas Flow	: 15 L/min (N_2)

Quantitative Analysis of Antioxidant

Additives such as antioxidants and static dissipators are contained in SAF. While the concentrations of various compounds in typical SAF are often in the percentage range, antioxidants like BHT (Butylhydroxytoluene) are regulated to around several tens of ppm in standards such as ASTM D2425. Therefore, the concentration of BHT is significantly different from that of SAF components, making it undetectable in Scan analysis of SAF components. However, by conducting measurements using FASST (Fast Automated Scan/SIM Type), it is possible to perform SIM analysis simultaneously during the retention time of BHT in addition to Scan analysis, allowing for the detection of BHT (Figure 4). When BHT was added to sample A at a concentration of 20 mg/L and a calibration curve was created using the external standard method, it was quantified at 19 mg/L, achieving a recovery rate of 95%.

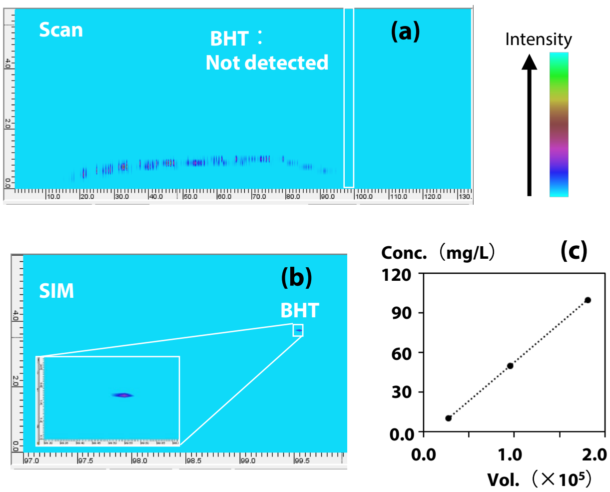

Fig. 4 FASST analysis of sample A
(a)Scan, (b)SIM, (c)Calibration curve
Analysis Condition: See Table2,
Event time : Scan (0.02s), SIM (*m/z* :205, 220, 0.01s)

Table 4 Analysis Conditions of diesel (Low polarity→Medium polarity)

GC	
1st Column	: SH-17 (P/N : 221-75907-30) (30 m × 0.25 mm I.D., df= 0.25 µm)
2nd Column	: SH-1 (P/N : 221-75723-30) (2.5 m × 0.32 mm I.D., df= 0.25 µm) *cut the column into 2.5 m
Injection Temperature	: 250 ˚C
Flow Control Mode	: Pressure (He)
Inlet pressure Program	: 20 kPa → 2.0 kPa/min → 220 kPa
Purge Flow	: 3 mL/min
Injection Volume	: 0.2 µL
Split ratio	: 100
Column Oven Temp. Program	: 40 ˚C → 2.0 ˚C/min → 240 ˚C
MS	
Ion Source Temperature	: 230 ˚C
Interface Temperature	: 280 ˚C
Measurement Mode	: Scan
Scan Range (*m/z*)	: 35-500
Event Time	: 0.02 s (= 50 Hz、 30,000 u/sec)
Modulator	
Modulation period	: 10 s
Hot pulse duration	: 350 ms (350 ˚C)
Cold Gas Flow	: 15 L/min (N_2)

Conclusion

Three SAF samples were measured using a combination of low-polar to medium polar columns and compared the two-dimensional images. The two-dimensional images allow for intuitive comprehension of the distribution of each component, making it easy to identify differences in composition and conducting quality control Inspection. Additionally, in the measurement of SAF using a combination of medium-polar to non-polar columns, the separation of paraffins and naphthenes was improved. Furthermore, by utilizing the FASST, composition analysis of SAF and quantitative analysis of antioxidants were simultaneously performed, which are regulated by concentration in ASTM D2425.

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<Related Applications>

1. Comprehensive Characterization of Diesel Fuel on GC×GC Utilizing Impressive High-Speed Scan Technology of GCMS-QP2050, Application News No.01-00788-EN

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