GCxGC data analysis of msFineAnalysis AI Ver. 3 ③Pyrolysis oil

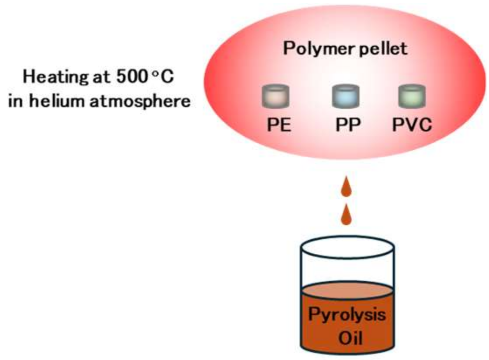
Product used: Mass Spectrometer (MS)

Introduction

The qualitative analysis software msFineAnalysis AI enables automatic structure analysis of unknown compounds not registered in libraries through EI/FI integrated analysis and AI structure analysis. Version 3 newly supports comprehensive 2D GC (GCxGC) data analysis. MSTips509 introduced the usefulness of EI/FI integrated analysis using diesel fuel analysis, and MSTips510 introduced the usefulness of AI structure analysis using polymer pyrolysis analysis. This MSTips introduces technique for comparing samples and identifying differential peaks using 2D chromatograms, using pyrolysis oil analysis. Pyrolysis oil is derived from discarded plastics and rubber products. It is used as an alternative fuel to petroleum and as a raw material for recycled plastics, making it one of the key technologies contributing to the circular economy.

Experiment

The pyrolysis oil sample was produced by mixing polyethylene (PE), polypropylene (PP), and polyvinyl chloride (PVC) pellets, then heating at 500° C for 15 minutes in a helium atmosphere. Figure 1 shows a schematic diagram producing pyrolysis oil a table of polymer pellet amount. The generated pyrolysis oil was washed away with chloroform and collected, and 1 µL of the diluted oil was injected into GC.



	Polyethylene (PE)	Polypropylene (PP)	Polyvinylchloride (PVC)
Pyrolysis oil ①	100 mg	0 mg	0 mg
Pyrolysis oil ②	50 mg	50 mg	0 mg
Pyrolysis oil ③	0 mg	100 mg	0 mg
Pyrolysis oil ④	45 mg	45 mg	10 mg

Figure 1 **Schematic diagram of producing pyrolysis oil and table of polymer pellet amount**

Table 1 Analytical conditions

Gas Chromatograph : 8890A GC (Agilent Technologies)	
Inlet temperature	300°C
1st column	BPX5 (TRAJAN) 30m, 0.25mm, 0.25µm
2nd column	Rxi-17Sil MS(Restek) 3.4m, 0.15mm, 0.15µm
Oven temperature	40°C(2min)-5°C/min -320°C(30min)
Split ratio	Splitless
Carrier gas	He, 2mL/min
GCxGC Modulator : INSIGHT-Thermal modulator (SepSolve Analytical)	
Modulation period	8 sec
Modulation loop length	77cm in 2nd column

Mass Spectrometer : JMS-T2000GC (JEOL)	
Ion Source	EI/FI combination ion source
Ionization	EI : 70eV
	FI : FI emitter, Flashing 12mA 3msec
IS temperature	EI : 250°C / FI : No heating
GC-ITF temperature	250°C
Mass range	*m/z* 30-800
Recording interval	EI : 0.02sec(50Hz) / FI : 0.04sec(25Hz)
Drift compensation	EI : PFTBA *m/z* 263.987, reservoir at end time
	FI : PDMS *m/z* 281.051, reservoir every 20min

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Results

Figure 2 shows the 2D chromatograms of pyrolysis oils ② (PE/PP) and ④ (PE/PP/PVC). In addition to the main components, the pyrolysates of PE/PP, trace components such as naphthalene and anthracene, which are the pyrolysates of PVC, could also be easily confirmed in the 2D chromatogram.

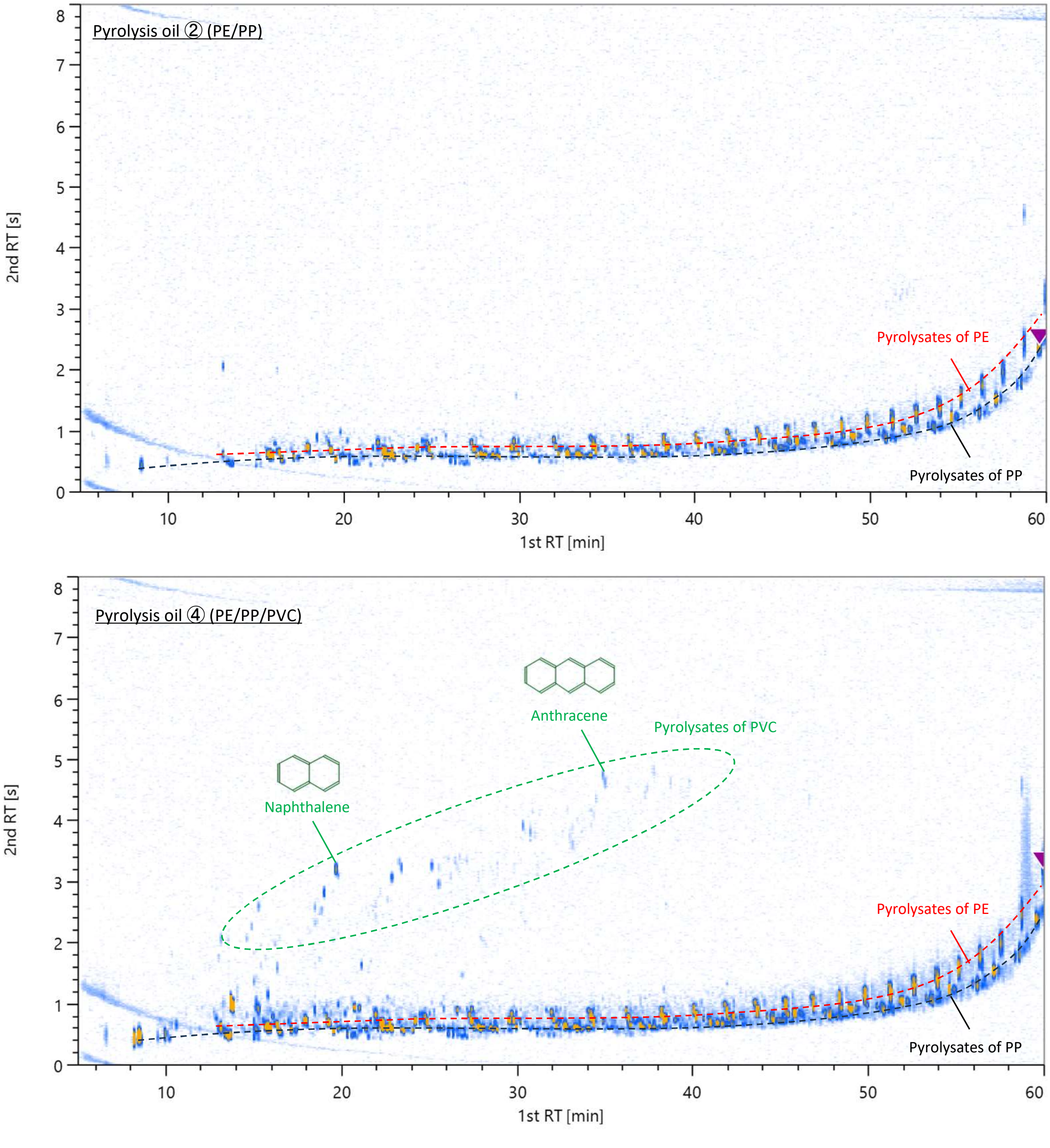

Figure 2 2D chromatograms of pyrolysis oil ② and ④

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Figure 3 shows enlarged 2D chromatograms of pyrolysis oils ① (PE), ② (PE/PP), and ③ (PP). Although the pyrolysis oils used in this study contained up to three types of base polymers, more than 200 peaks were detected. The 2D chromatograms obtained by GCxGC-MS allowed for clear separation and detection of these numerous peaks, and the peak distribution made it easy to infer compound structures.

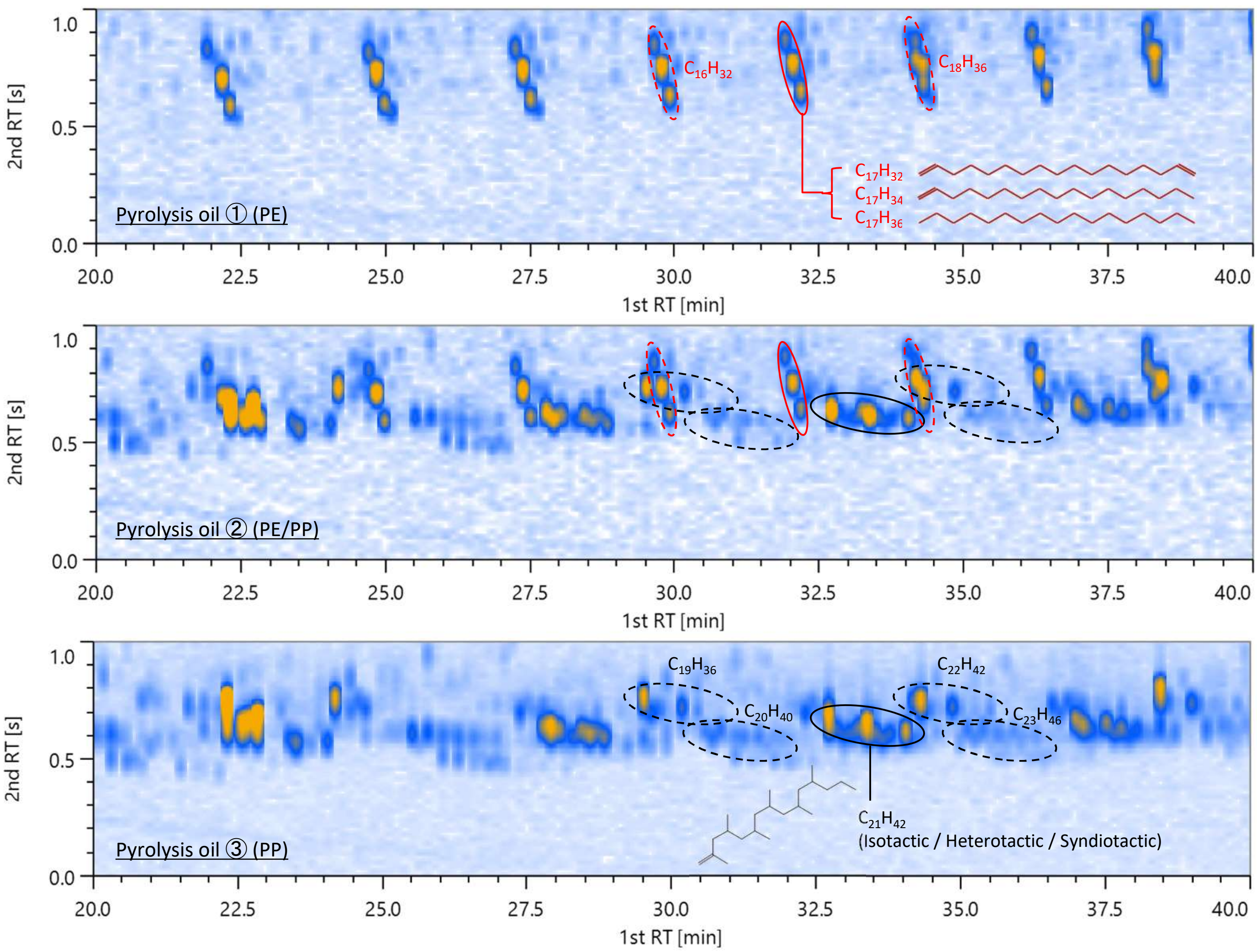

Figure 3 2D chromatograms of pyrolysis oil ①, ②, ③ (Enlarged view)

Conclusion

With the new support for GCxGC data analysis in msFineAnalysis AI Ver.3, it is now possible to visualize qualitative information from complex samples such as pyrolysis oils and to quickly compare multiple samples.

Acknowledgement

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