

Group-type analysis of Crude Oil using GC/FI-TOFMS 1

~Determination of average molecular weights by group-type analysis~

Introduction

Field Desorption (FD) and Field Ionization (FI) are ionizing analytes by electron tunneling from analyte molecules to the solid surface (emitter) in a high electric field. In case of FD, the sample is applied on the emitter and heated by applying an electric current through the emitter for desorption and ionization. In the case of FI, vaporized analyte molecules are introduced to the proximity of the emitter.

FI is a soft ionization method that yields intact molecular ions and in most cases, with very few fragment ions. It was used to ionize analytes that are easy to fragment and where molecular ions are difficult to be detected, such as hydrocarbons in crude oil.

For complex mixtures such as crude oil or synthetic polymers, molar mass distributions and average molecular weights are important chemical properties. By analyzing a FI mass spectrum, mostly consisting of molecular ions of complex hydrocarbon mixture, and using a group-type analysis software, one can obtain molar mass distributions and average molecular weights of the various hydrocarbon types (e.g., paraffin, naphthene, olefin, aromatics) in the mixture.

We have analyzed a crude oil sample by GC/FI method using JMS-T100GC "AccuTOF GC" and processed the obtained data using a group-type analysis software.

Methods

Sample Crude Oil

(Refer Fig. 1 for preparation)

Analysis conditions

GC conditions

GC:	Agilent 6890N
Column:	DB-5ms 30 m x 0.25 mm I.D., 0.25 μ m
Oven:	50°C → 15°C/min → 280°C (5 min)
Injection port:	280 °C, Split (1:200)
Injection volume:	1.0 μ l
Career gas:	He (1 mL/min, constant flow mode)

MS conditions

MS:	JMS-T100GC "AccuTOF GC"
Ionization:	FI+ (Cathode voltage: -10 kV, Emitter current: 0 mA)
Mass range:	m/z 35 - 500
Acquisition rate:	0.3 s/spectrum

Software Polymerix™ (Sierra Analytics, Inc.)

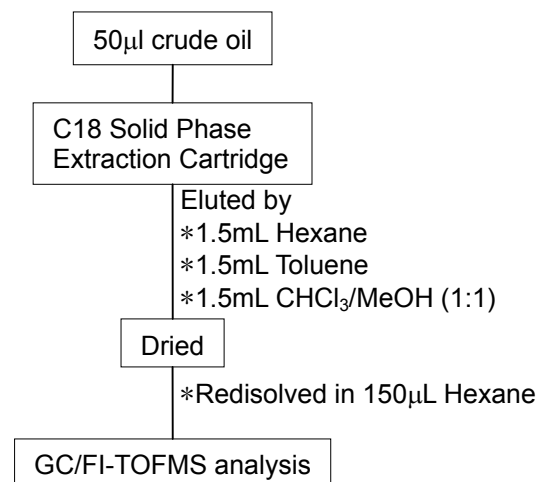
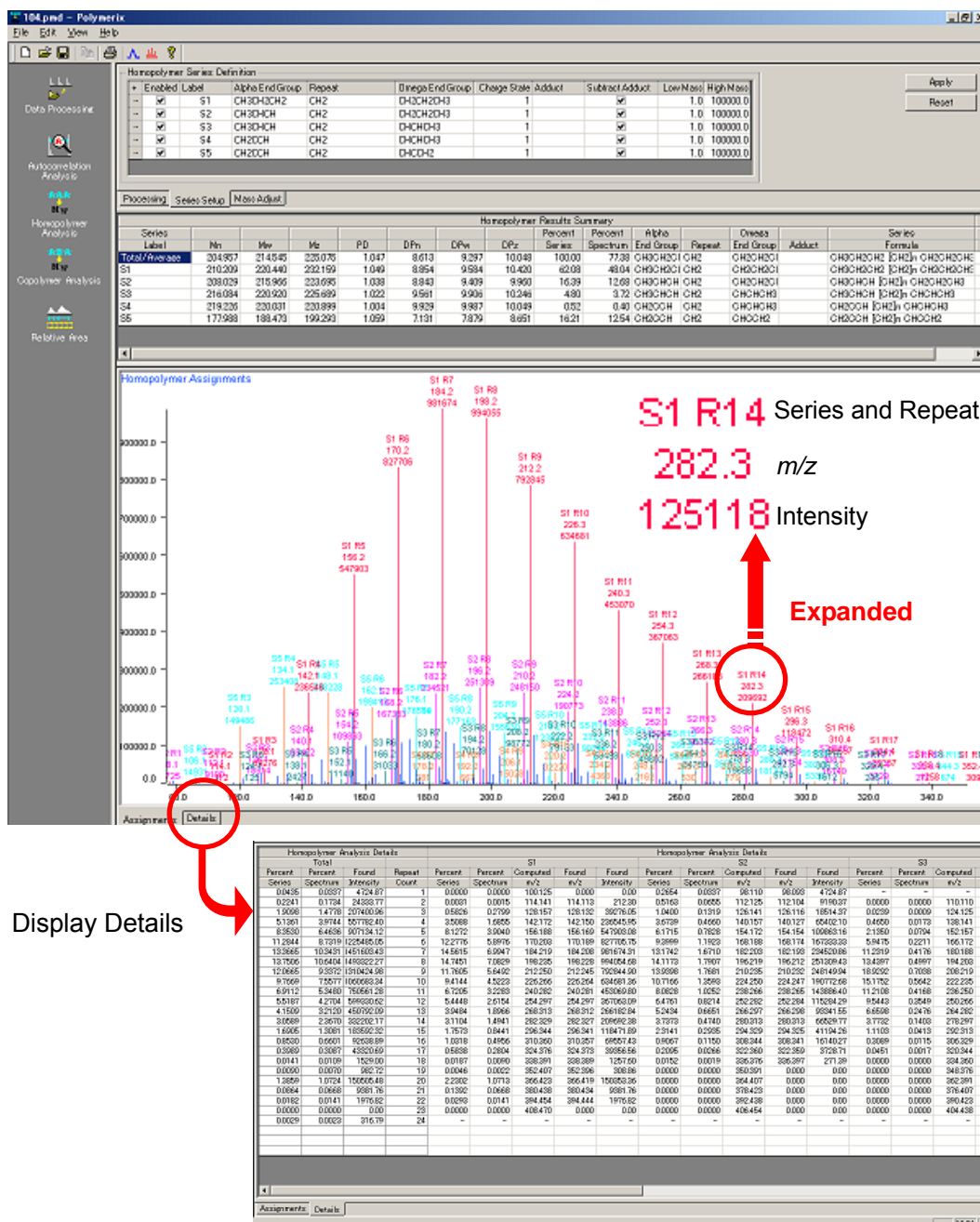


Fig. 1 Sample preparation flow

Results and Discussion

The output from the group-type analysis software Polymerix™ (Sierra Analytics, Inc., <http://masspec.com/>) is shown in Fig. 2.



- Specify α and ω end groups and repeating unit.
- Perform group-type analysis.
- Results such as M_n , M_w , M_z , and polydispersity for each series are displayed.
- Mass spectral peaks are color coded based on the series to which they belong.

Display Details

Fig. 2 The group-type analysis results of the Crude Oil

The data acquired by the AccuTOF GC was directly read into the Polymerix™ software. All the mass spectra acquired during the retention time range of the sample were summed to form a single mass spectrum and then processed. Properties such as number average molecular weight (M_n), weight average molecular weight (M_w), z average molecular weight (M_z), and polydispersity (PD) were calculated for 5 hydrocarbon types with the degree of unsaturation from 0 to 4 and for the total/average of the 5 types.

Group-type analysis of complex hydrocarbon mixtures such as crude oil can be easily performed by using GC/FI method on the AccuTOF GC and Polymerix™ group-type analysis software.