

Analysis of heavy oil components with Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS)

Japan Petroleum Energy Center

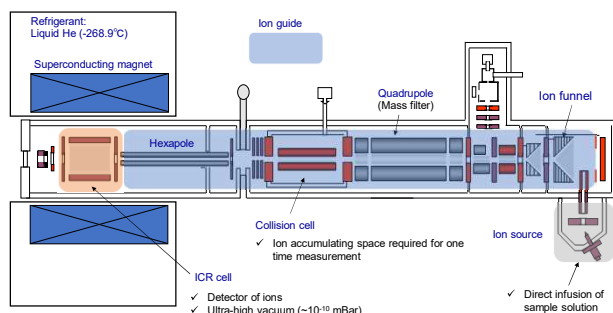


What's FT-ICR MS?

Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS)

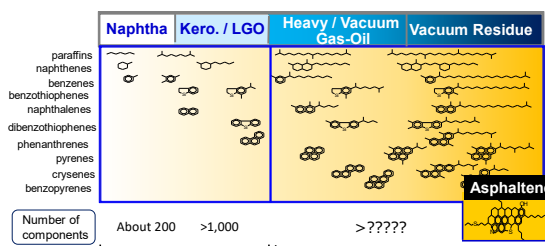


- ✓ FT-ICR MS is high-resolution technique that can be used to highly-complex mixtures.
- ✓ Petroleum science field based on molecular level information provided by FT-ICR MS is called "Petroleomics".
- ✓ JPEC is the only research institute applying FT-ICR MS to oil analysis in Japan.



- ✓ Ultimate way to increase resolving power of FT-ICR MS is to increase the strength of magnetic field.
- ✓ High field (12 Tesla) is appropriate for analysis of heavy oil sample.

Features of Analysis



- ✓ Conventional analysis techniques (GC, GC × GC) are available.
- ✓ Target of FT-ICR MS
- ✓ Detailed information of high boiling fraction over 360°C is essential to understand underlying chemistry of the upgrading process.

Conventional analysis

Sulfur	Whole sulfur content
Nitrogen	Whole, basic or neutral nitrogen content
Molecular structure	AVERAGE structure by using NMR, distillation, MS, GPC, C/H ratio etc.

Petroleomics (FT-ICR MS)

Structure and amount of sulfur containing core
Structure and amount of nitrogen containing core
Core, bridge and chain structure of All molecules

- ✓ Petroleomics technology gives molecular level structural information, especially aromatic and naphthenic ring structure.

➢ Heavy oil components are analysed with this method.

Light oil like as Kerosene, Gasoil, Plastic recycle oil and Biomass oil are not covered.

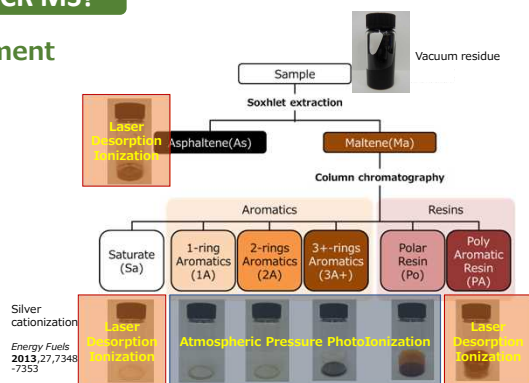
➢ Carbon number/molecular weight range

: Carbon number 14~100/ molecular weight 250~1200

➢ Analysis target : Hydrocarbon as oil (Sa, 1A, 2A, 3A+, Po, Pa, As), N, S, O, V

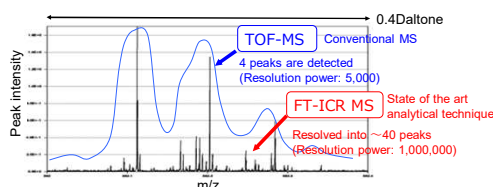
What's FT-ICR MS?

① Pretreatment



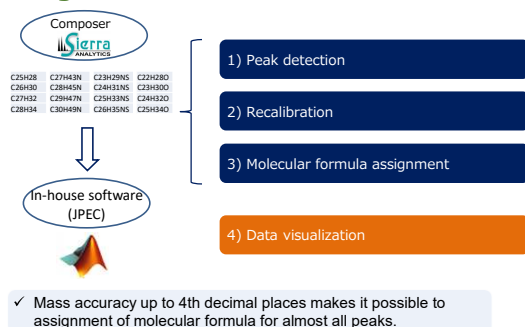
- ✓ The sample is separated into 7 fractions as pretreatment.

② FT-ICR MS



- ✓ Ultra-high resolving power reveals fine structure of isotopic peaks.

③ Processing



Output

① Molecular formula assignment

[List of all components]
Tens of thousands of molecules can be detected.

	C	H	N	O	S	molecular formula
1	14	12	0	0	1	C14H12S
2	15	12	0	0	1	C15H12S
3	15	13	1	0	0	C15H13N
4	15	14	0	0	1	C15H14S
43	17	17	1	0	0	C17H17N
44	17	17	1	1	0	C17H17NO
45	17	18	0	0	0	C17H18
46	17	18	0	0	1	C17H18S
13424	93	120	0	0	0	C93H120
13425	93	129	1	0	0	C93H129N
13426	94	108	0	0	0	C94H108
13427	94	118	0	0	0	C94H118

② Data visualization

