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I am Intertek UK's Sustainable Hydrocarbon Specialist, primarily concerned with the analysis of complex matrices for which methods do not necessarily exist. Personally I have over 15 years' experience conducting chromatography on organic sample, and collectively team have been assisting clients understand the composition of hydrocarbon samples for over twenty years.

I have a Masters in Analytical Chemistry from Loughborough University



(GCxGC) Field Desorption Time of Flight Mass Spectrometry

Method description in brief.

A sample is separated by liquid chromatography into saturates and aromatics before introduction to a time of flight mass spectrometer using a field desorption filament.

The resultant mass spectra is dominated by molecular fragments due to the soft ionisation. This can be processed into a matrix of carbon number by degree of saturation using the accurate mass (4dp).

The individual saturation numbers (hydrocarbon classes) are then summed, and factored up to the whole sample using the separation data.

A GCxGC sample introduction technique is under development but it is not expected to that validated data will be available in time for production of the poster.

Applicability of method.

The Intertek FD-TOF-MS method capable of determine the hydrocarbon composition of complex matrixes with a limit of detection of 0.01wt%.

Results for each fraction are split into a matrix of Carbon Number by Degree of Saturation as shown below

Parameter	Range
Carbon Number	C10-C120
Degree of Saturation	Saturates: 2 to -24 Aromatics: -6 to -46

Sample preparation required.

Samples need to be separated into Saturates and Aromatics usually by means of Liquid Chromatography.

A GCxGC front end for the FD-TOFMS is under development.

Method strengths.

The method utilizes well characterised separation techniques and combined this with the power of the Time of Flight mass spectrometer. High mass resolution and accurate mass data allows for the deconvolution of complex matrices via a relatively simple introduction method. If the sample can be separated it can be analysed.

Estimated time for analysis.

Sample Preparation: Dependant on sample type, IP368 of lube oil typically ~2 hours

Analysis: 5 minutes per fraction, 10 minutes for Sats and Aromatics

Data Processing/Interpretation: 1-2 hours depending on complexity of sample

Method weaknesses.

1. Field desorption is a magnitude of sensitive higher than EI, therefore limits of detection of in the region of 0.01 wt%
2. A mobile phase is required for the LC separation therefore samples need an IBP significantly away from solvents such as hexane or heptane so the solvent can be blown down or distilled off. We are working on a GCxGC front end of the analysis to remove this weakness for lower boiling products.

Result interpretation / visualisation / presentation.

A presentation is attached which was presented to Concawe in 2022



Concawe FDMS.pdf

Relevant Papers

No specific papers, Intertek has analysed and reported a number of samples for Concawe over a significant period of time.