Enhanced Simulated Distillation Analysis with Slice Report: Leveraging the Power of GCxGC

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Introduction

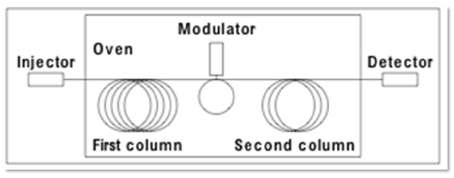
Simulated distillation (SimDist) is a critical analytical technique in the oil industry, providing detailed insights into the boiling point distribution of crude oil and its fractions. While traditional gas chromatography (GC) has been the standard, it often faces limitations in resolving complex hydrocarbon mixtures, particularly in heavy fractions. Comprehensive two-dimensional gas chromatography (GCxGC) provides significant advantages over one-dimensional GC by greatly improving the separation of complex hydrocarbon mixtures. When combined with the tailored data processing capabilities of software tools, this approach improves the precision and reliability of SimDist results, empowering refineries to optimize both process and product quality.

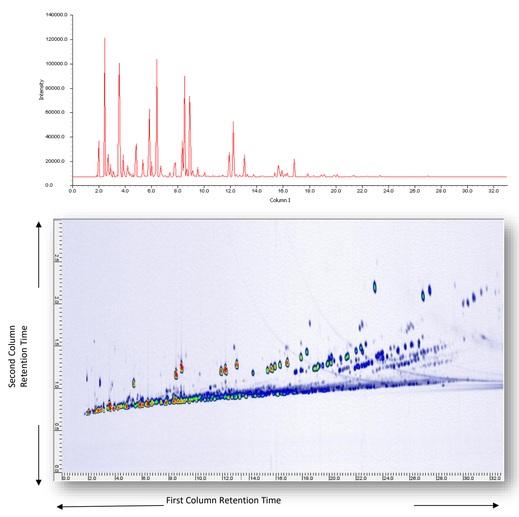
Power of GCxGC

Comprehensive two-dimensional gas chromatography (GCxGC) provides significant advantages over one-dimensional GC, including:

- Greatly improved the separation of complex hydrocarbon mixtures;
- Accurately resolving overlapping components into individual group of compounds;
- Detecting trace compounds and column bleeds

, which allow obtaining a more detailed and reliable boiling point distribution curve.





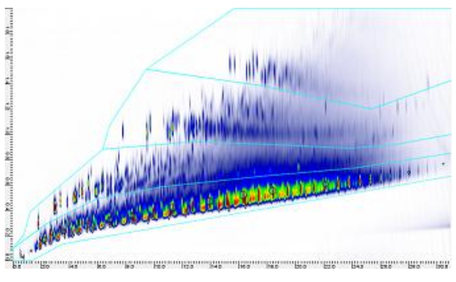
Data Processing

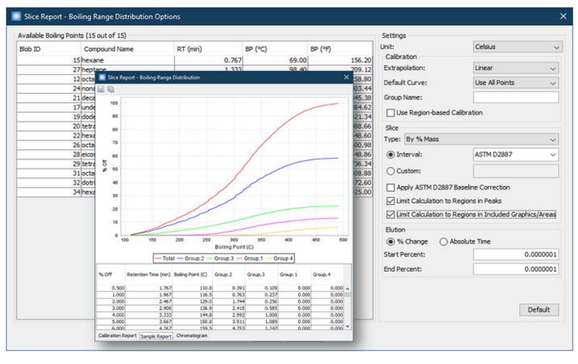
Leveraging the 2D separation power of GCxGC, GC Image Software [1] provides a comprehensive set of tools, specifically designed to enhance the analysis of boiling range distributions:

❖ **Tailored Baseline Correction**: The software is able to locate background regions in the two-dimensional separation space automatically and provides an accurate baseline estimation.

❖ **Enhanced Accuracy with 2D Separation**: The software can restrict calculations to detected peaks or custom graphics and areas, which allows removing background noise and interferences more precisely.

❖ **Comprehensive Group Analysis**: The software has the ability to generate distribution curves for individual group of compounds that are defined by sophisticated graphical objects in the 2D retention-time space.





Sample Analysis

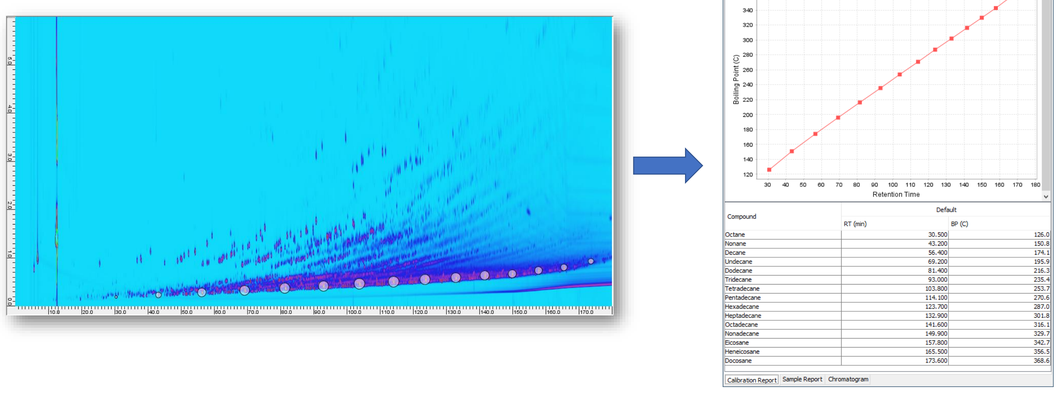
A diesel fuel sample was collected from a commercial gas station in Houston, TX, USA. The sample was diluted 1:10 in dichloromethane and injected directly into a GCxGC/FID system without further preparation. The instrument parameters are listed in Table 1.

Table 1. Instrument Parameters

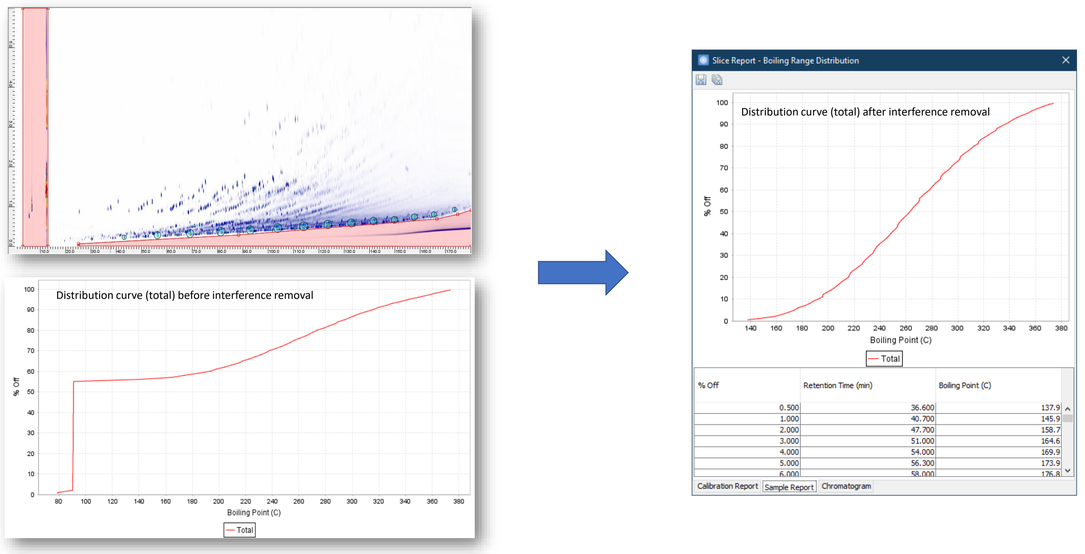
GC/FID	Agilent 6890
GC x GC system	Dual stage delay loop thermal modulator
1st column	DB-1, 30m x 0.25mm, 0.25µm
2nd column	DB-Wax, 1.3m x 0.1mm, 0.1 µm
Modulation loop	DB-Wax, 1.3m x 0.1mm, 0.1 µm
Modulation period	6 s
Inlet mode	Split ratio 200:1, Ramp pressure
Oven temp.	40 °C -> 1.2 °C/min -> 240 °C
Inlet pressure	35 PSI-> 0.2 PSI/min -> 65 PSI
Inlet temperature	280 °C
FID temp.	300 °C
Acquisition rate	100 Hz

Results

Calibration: A boiling point calibration curve is generated using normal paraffin peaks (C8 – C22) detected in the sample.



Interference Removal: Solvent, its impurities, and column bleeds are excluded through the use of graphical objects.



Group Analysis: Distribution curves are generated for the three groups defined by the UOP 965 method [2].

Reference

[1] GC Image v2024. https://www.gcimage.com/docs/index.html
[2] ASTM UOP965-10, “Total Cycloparaffins and Total Aromatics in Synthetic Paraffinic Kerosene Fuels by Comprehensive Two-Dimensional GC with Flame Ionization Detection”. https://www.astm.org/uop965-10.html

InfoMass LLC

GC Image
Software for Multidimensional Chromatography