Group-type quantitation of hydrocarbons in aviation fuel using GC×GC–FID

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Introduction

Accurate hydrocarbon composition of finished fuels, such as aviation fuel, is required to ensure quality control and to determine the effects of processes in fuel production. This has become even more important with the development of novel renewable fuels, such as sustainable aviation fuels (SAFs).

Here, we demonstrate the use of reverse fill/flush (RFF) flow-modulated GC×GC–FID and automated group-type data processing to provide fast and accurate quantitative information on hydrocarbon composition.

Experimental

Samples: A reference standard and reference blends of both diesel and aviation turbine fuel.

GC×GC: Modulator: INSIGHT®-Flow reverse fill/flush (RFF) flow modulator (SepSolve Analytical); Modulation period (P_M): 7.8 s. Carrier gas: H_2.

Column set: ASTM D8396 reverse phase column set (SepSolve Analytical, PN: OEM-SEP-COLKIT-10)

FID: Total H_2 flow (column & fuel): 50 mL/min; Air flow: 350 mL/min; Makeup gas flow: 5 mL/min; Temperature: 300 °C.

Software: ChromSpace® GC×GC software for instrument control and data processing.

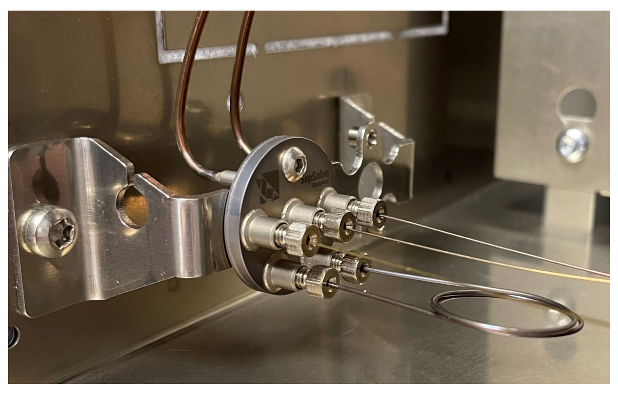


Figure 1: The INSIGHT-Flow modulator used in this study.

Results and discussion

Optimising the GC×GC separation

Separation was optimised using a custom column set and larger loop volume, enabling excellent separation of the key chemical classes (Figure 2).

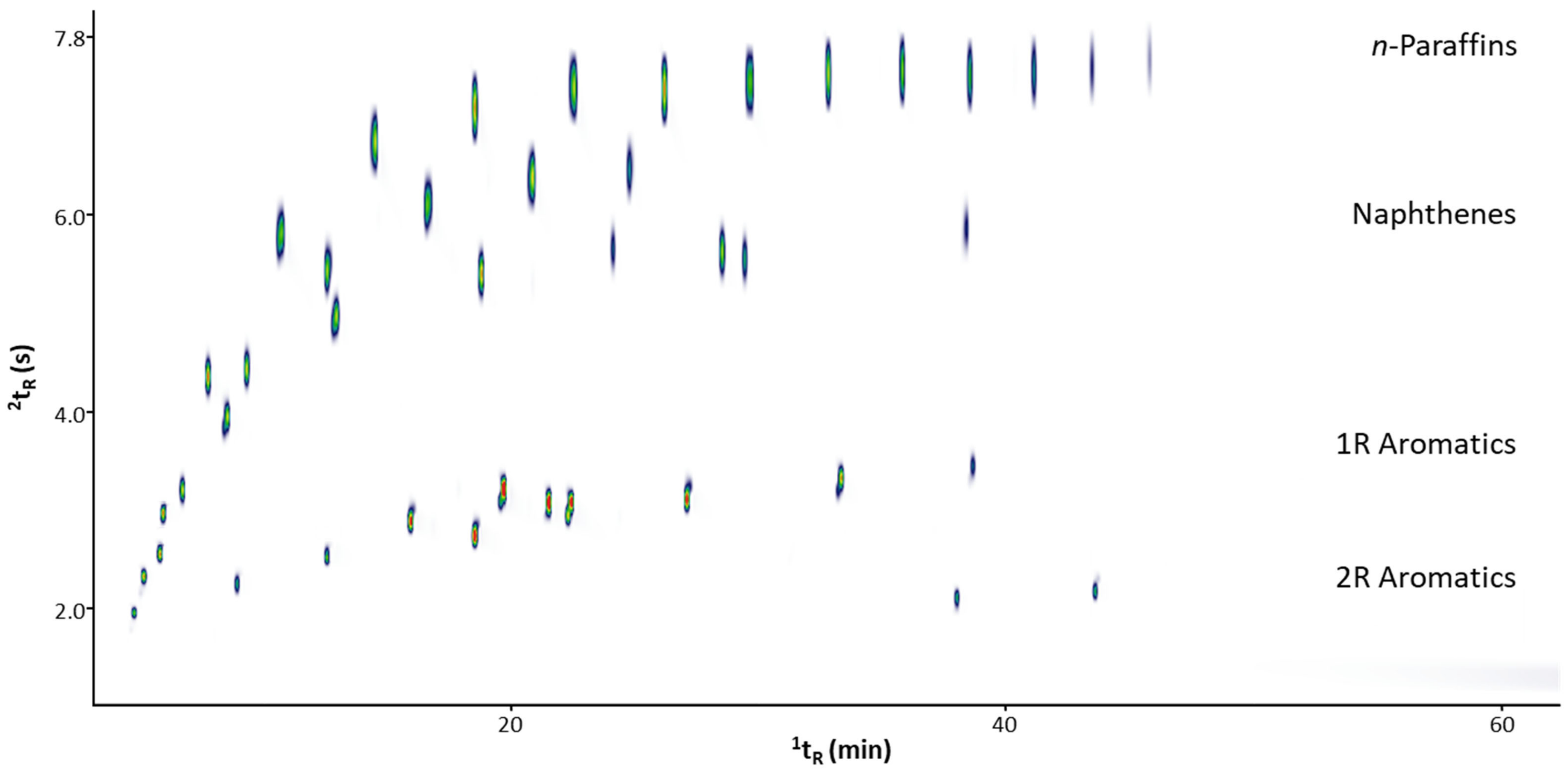


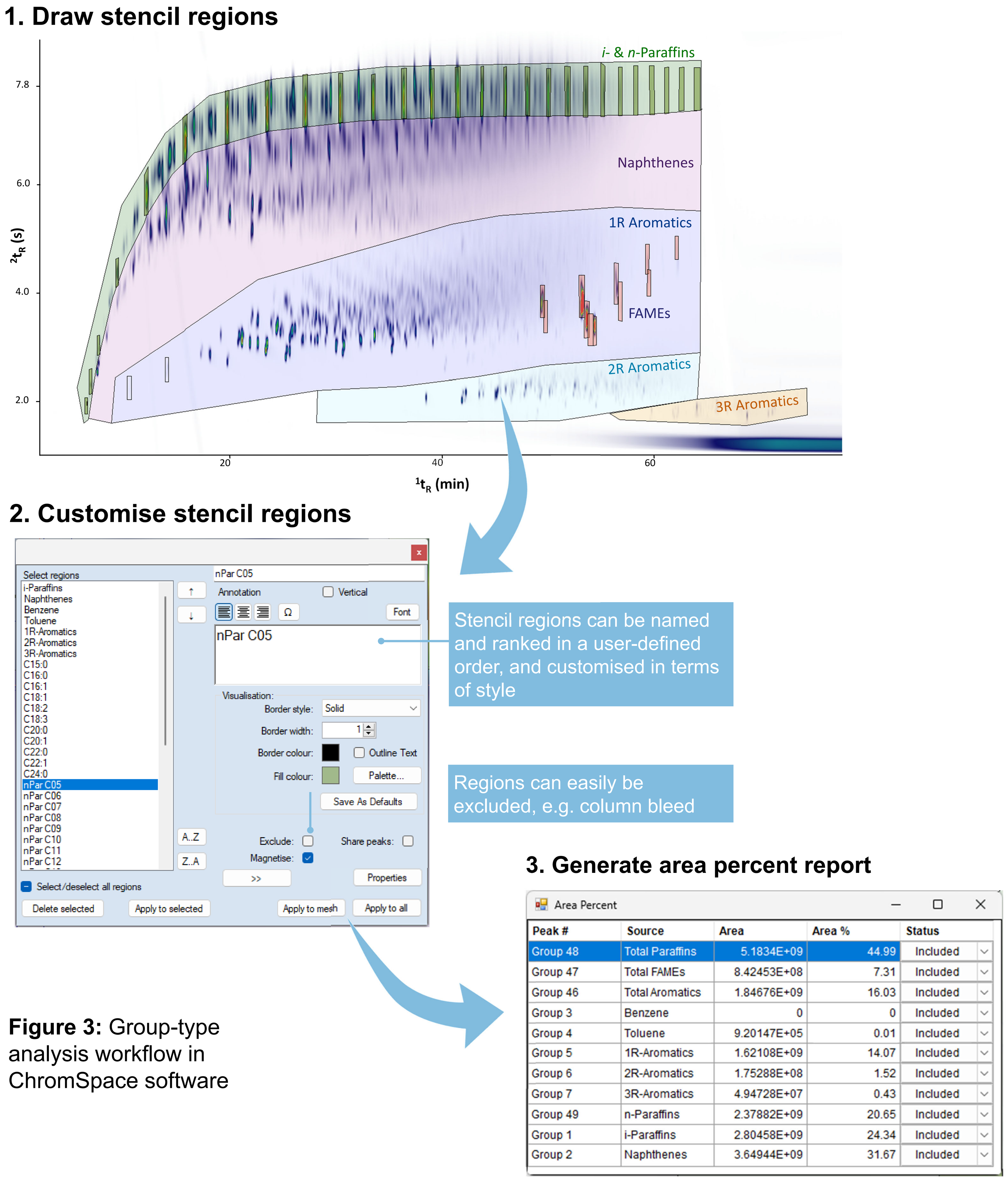
Figure 2: GC×GC–FID colour plot for the separation of a reference standard containing the chemical classes of interest.

The INSIGHT-Flow modulator used in this study has an adjustable sample loop (in the range of 25-250 µL) for greater flexibility in method development. The reference standard was analysed in replicate (n=10) to assess method repeatability and precision. The relative standard deviation (RSD) of the raw peak areas were all <2%, while the calculated mass percent values were consistently within 0.5% of the known composition.

Group-type classifications

Group-type analysis of these key chemical classes was then performed on various fuels using the 'stencil' workflow in ChromSpace software (Figure 3).

Once a stencil is created, it can be saved and applied to multiple data files in an automated batch sequence to generate area percent reports. This means that the method is then scalable across multiple GC×GC–FID platforms for fast classification. This proven workflow has already gained accredited status in a number of high-throughput environmental labs for the analysis of total petroleum hydrocarbons (TPH).



Peak #	Source	Area	Area %	Status
Group 48	Total Paraffins	5.1834E+09	44.99	Included
Group 47	Total FAMEs	8.42453E+08	7.31	Included
Group 46	Total Aromatics	1.84676E+09	16.03	Included
Group 3	Benzene	0	0	Included
Group 4	Toluene	9.20147E+05	0.01	Included
Group 5	1R-Aromatics	1.62108E+09	14.07	Included
Group 6	2R-Aromatics	1.75288E+08	1.52	Included
Group 7	3R-Aromatics	4.94728E+07	0.43	Included
Group 49	n-Paraffins	2.37882E+09	20.65	Included
Group 1	i-Paraffins	2.80458E+09	24.34	Included
Group 2	Naphthenes	3.64944E+09	31.67	Included

Figure 3: Group-type analysis workflow in ChromSpace software

Improving productivity with dual channel GC×GC–FID

Additionally, two INSIGHT-Flow modulators can be configured within the same GC oven (Figure 5) to enable simultaneous analysis of two samples in a dual-channel mode. Importantly, the dual-channel system is fully controlled using ChromSpace, with reporting of data from both channels performed automatically.

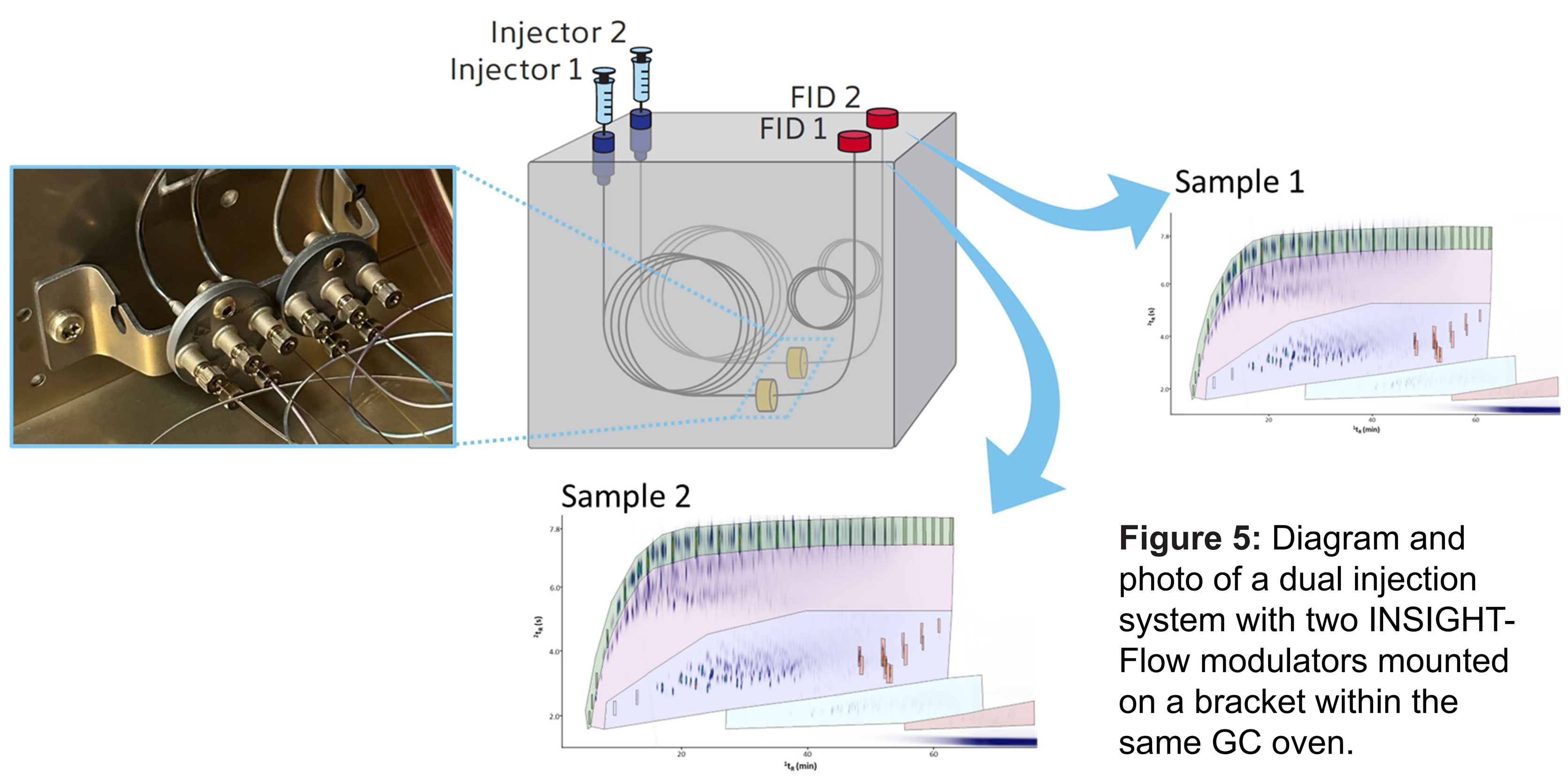


Figure 5: Diagram and photo of a dual injection system with two INSIGHT-Flow modulators mounted on a bracket within the same GC oven.

Conclusions

This poster has shown an end-to-end workflow for ASTM Method D8396, specifically:

- Proven reverse fill/flush modulation using the INSIGHT-Flow, a modulator in operation in numerous high-throughput labs across the world.
- Optimal class separation with a tried-and-tested column set.
- Fast, straightforward group-type data processing with ChromSpace software.
- Doubled productivity with optional dual-channel GC×GC technology.
- A retrofittable solution for all popular GCs, allowing existing systems to be upgraded to GC×GC capability.

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