GC×GC method translation from thermal to differential-flow modulation: when expectations become reality

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Abstract

Comprehensive two-dimensional gas chromatography GC×GC coupled with mass spectrometry (MS) is a powerful technique for detailed profiling and effective fingerprinting of medium-to-high complexity samples. Thermal modulators (TMs) implementing cryogenic cooling are widely used and, to date, considered as a "golden standard" for GC×GC. The effective band focusing-in-space generated by this modulator results in a peak capacity gain (G_n) that is close to the achievable theoretical limit [1]. At the same time the signal-to-noise ratio greatly increases resulting in a sensitivity gain of one order of magnitude compared to a conventional 1D-GC analysis. Despite these advantages, thermal modulators have some drawbacks related to hardware and operational costs limiting their widespread adoption in quality control and high-throughput screening.

Differential-flow modulators (FMs) are an interesting alternative to TMs. FMs based on the original device proposed by Seeley *et al.* [2] have a simple and effective design, low operational and hardware costs, and high robustness. Commercial devices for FM GC×GC implemented with a Capillary Flow Technology (CFT) microfluidic plate and involving the reverse fill/flush (RFF) injection [3] provide highly efficient band re-injection, improved ^{2}D peak-widths and symmetry, and effective handling of collection-channel overloading. System performance was demonstrated in flavor and fragrance applications and heavy petroleum cuts.

This study investigates the applicability of method translation principles [4] to GC×GC for an effective translation of methods from TM to FM platforms that addresses also several challenges: (a) preservation of the 1D elution order, peak capacity, and resolution of the targeted/original method; (b) generation of coherent 2D peak patterns; (c) reliable transfer of metadata by a pattern recognition approaches; and (d) method sensitivity and information power. Results are presented for two model mixtures of interest for fragrance and aroma applications and rationalized for method sensitivity (absolute and relative), separation capacity, and 2D-peaks pattern coherence.

References

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