

# Utilizing GCxGC for Advanced Analytical Analysis of Volatile and Semi-Volatile Organic Compounds

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## Abstract

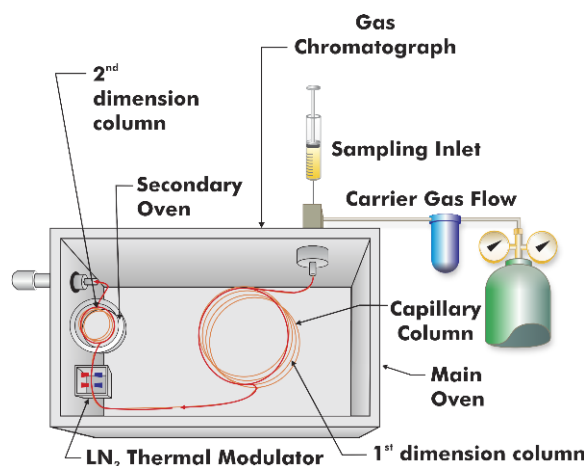
Volatile and semi-volatile organic compounds are some of the most widely studied samples. Traditional analytical methods rely on single dimension gas chromatography (GC) coupled to selective detectors or mass selective detectors (MS). More recently, the use of comprehensive two-dimensional gas chromatography (GCxGC) as an advanced analytical tool has gained significant popularity for complex sample analysis, target species in a heavy matrix, screening of difficult samples and quantification of compounds below traditionally reported L.O.D's. Recent advances to GCxGC instrumentation have made this technique more applicable to field analysis and the possibility of future space applications. This presentation will focus on GCxGC and explore the opportunities that make it a viable tool for advanced analytical analysis on future space missions.

## 1. Introduction

Since its invention just over a decade ago, the novel technique of comprehensive two-dimensional gas chromatography (GCxGC) has been developed to separate and analyze complex samples such as petroleum<sup>1-5</sup>, flavors<sup>6</sup>, environmental<sup>7-9</sup> and even human breath samples<sup>10</sup>. The technique of GCxGC employs two coupled columns of different selectivity and subjects the entire sample to a two-dimensional separation. Effluent from the primary column is modulated to produce sharp chemical pulses, which are rapidly separated on the second column. A separation plane is produced by the two orthogonal retention time axes for the columns<sup>11</sup>. Usually, the first column contains a non-polar stationary phase and the second column a polar stationary phase. This combination allows components to be independently separated, first according to their volatility and then according to their polarity. In comparison to conventional single-column gas chromatography, GCxGC has much higher peak capacity because the available peak

capacity is the product of the peak capacity of both dimensions. Other advantages of GCxGC include enhanced detectability due to analyte refocusing, true background around resolved peaks, more reliable identification due to two retention times and well ordered bands of compound groups<sup>12</sup>. The key element in a GCxGC system is the modulator, which focuses segments of the effluent from the primary column and re-injects them onto the secondary column.

### 1.1 Schematic of GCxGC

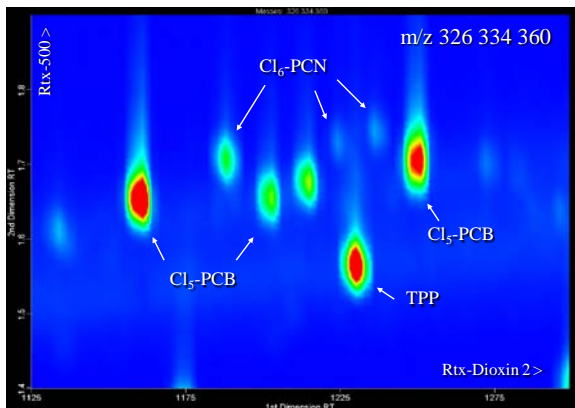


*Figure 1. Schematic of a GCxGC system showing 1<sup>st</sup> dimension column, thermal modulator and 2<sup>nd</sup> dimension column located inside a secondary oven.*

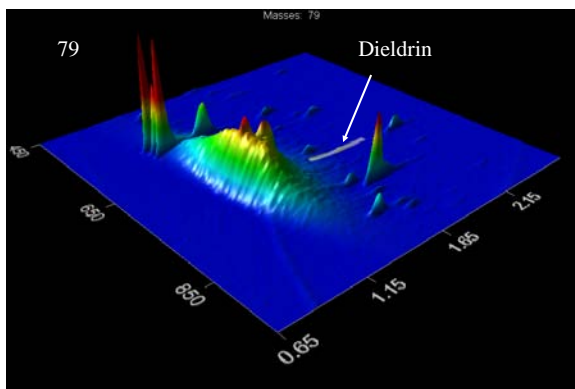
## 2. Applications for GCxGC

GCxGC is widely known as an advanced analytical tool for complex sample analysis. Over the last ten years multiple review papers have been published and the number of research groups and relevant applications is increasing steadily. Of significant importance is the contribution of GCxGC to the fields of environmental analysis (trace level detection of P.O.P's), petroleum (sulfur speciation and fingerprinting), food and flavors (off-flavor

compounds and batch processing) as well as metabolomics (human breath, biomarker discovery, plant and animal small molecule analysis). Relative to the field of space science, the analysis of meteorite fragments, planetary soil and dust analysis as well as the study of primordial soups can be explored by GCxGC. The examples below highlight the features that GCxGC offers for complex sample analysis.



**Figure 2.** GCxGC contour plot of PCB's and PBN's in a fish extract.



**Figure 3.** GCxGC analysis, identification and quantification of Dieldrin in a cucumber extract sample.

### 3. Summary and Conclusions

The use of GCxGC for complex sample analysis, trace level detection of target compounds and advanced screening of biological samples has become a viable tool for analytical researchers. Key advantages such as increased peak capacity, enhanced resolution and increased detectability are essential for trace level identification and screening

in complex matrices. Advances in sample collection systems, modulators and high speed detectors have aided in the use of GCxGC as a more routine technique. Further work aimed at eliminating consumables and decreasing footprint size will make GCxGC applicable to future space missions.

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