Characterisation of an Oil Contaminated Soil using GCxGC-ToF-MS

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Introduction

- Chemical characterisation of a soil contaminated with aviation fuel oil represents a vital step in the development of an effective remediation strategy.

- Information on the chemical composition of such complex mixtures is used, as part of a risk assessment, to assess the toxicity and subsequently identify the most suitable technology for treatment.

- Currently, analyses of these complex samples is conducted using standard protocols based on gas chromatography with flame ionisation (GC-FID) or in a few cases mass spectrometry (GC-MS).

- A common feature of gas chromatograms (GC) of soil contaminated fuel oil samples, especially when weathered, is the presence of an unresolved complex mixture (UCM, Fig 1).

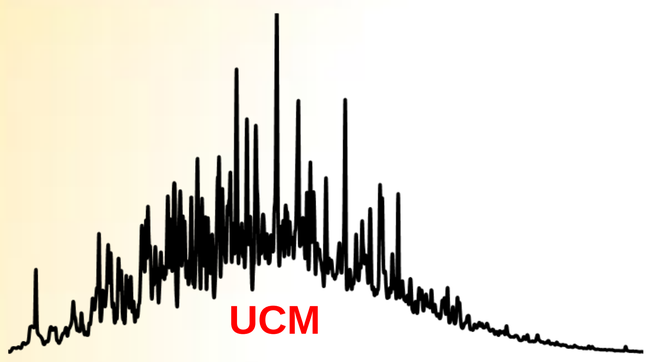


Figure 1. GC-MS mass chromatogram of a soil contaminated with aviation fuel oil.

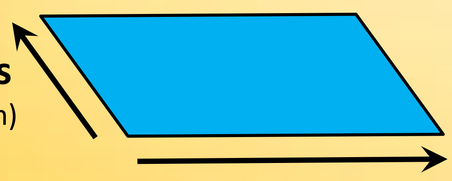
- The UCM concentration typically far exceeds the concentrations of the limited number of individual priority pollutants which conventional methods can characterise.

- In the present study we report the application of comprehensive gas chromatography-time of flight-mass spectrometry (GCxGC-ToF-MS) for the analysis of a soil sample taken from a site contaminated by aviation fuel oil.

Materials & Methods

Contaminated Soil Sample
(**T**otal **O**rganic **E**xtract or TOE)

GCxGC-ToF-MS
- 1μL TOE injected into 280°C splitless injector
- Oven program from 40 to 250°C @ 5°C min^{-1}, then hold for 10min



2nd Column: VF-23ms
(2m x 0.1mm i.d x 0.1μm film)

1st Column: HP-5ms
(30m x 0.2mm i.d x 0.25μm film)

Acknowledgments

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Results

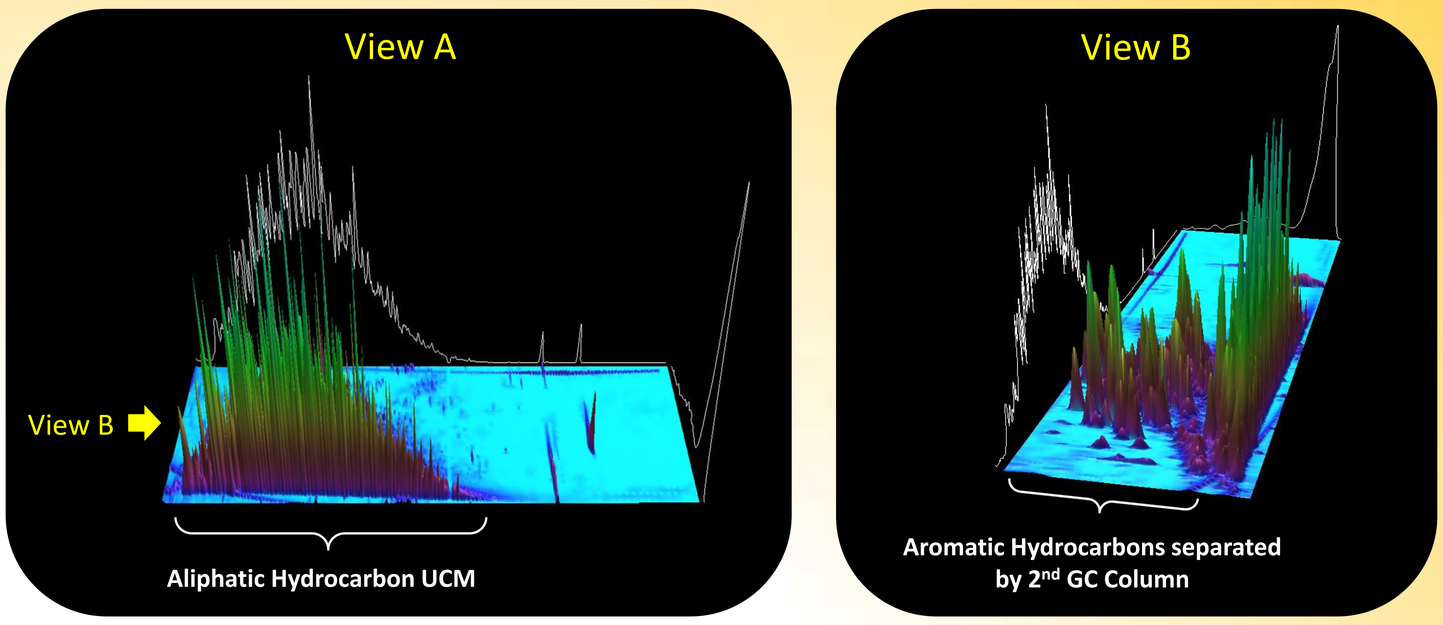


Figure 2. GCxGC-ToF-MS Total ion mass (TIC) chromatogram of a soil contaminated by aviation fuel oil.

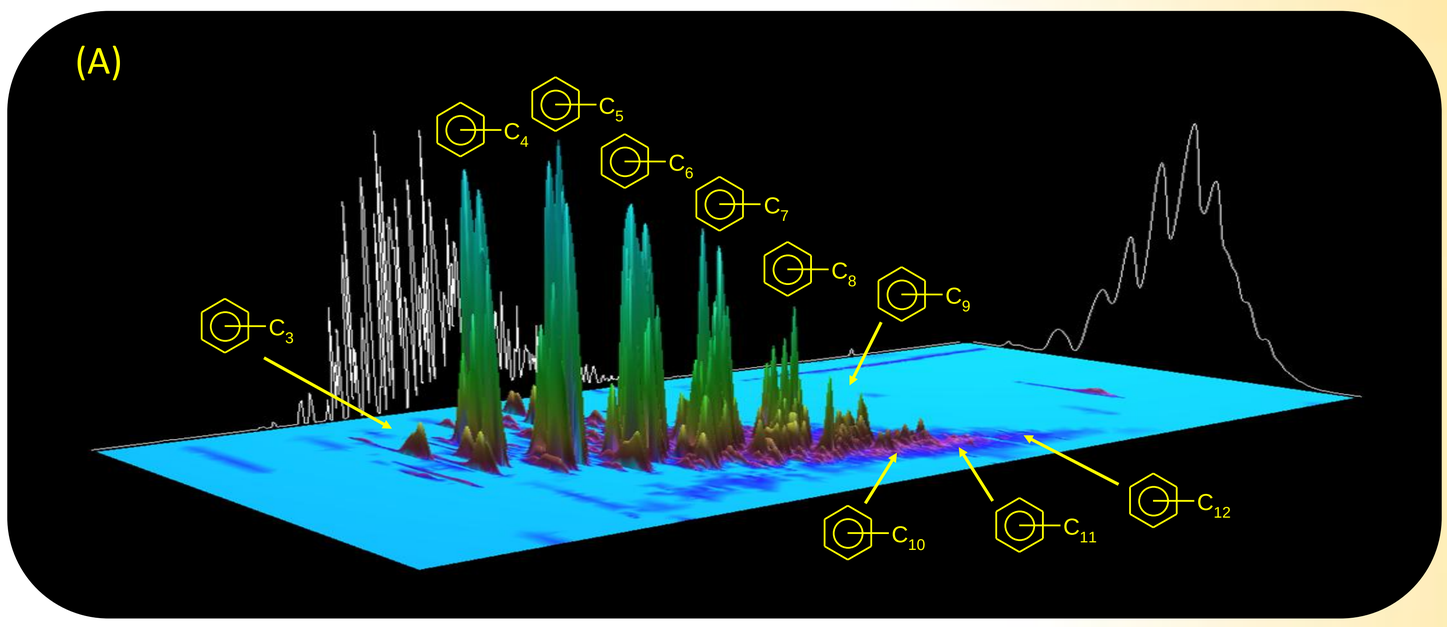
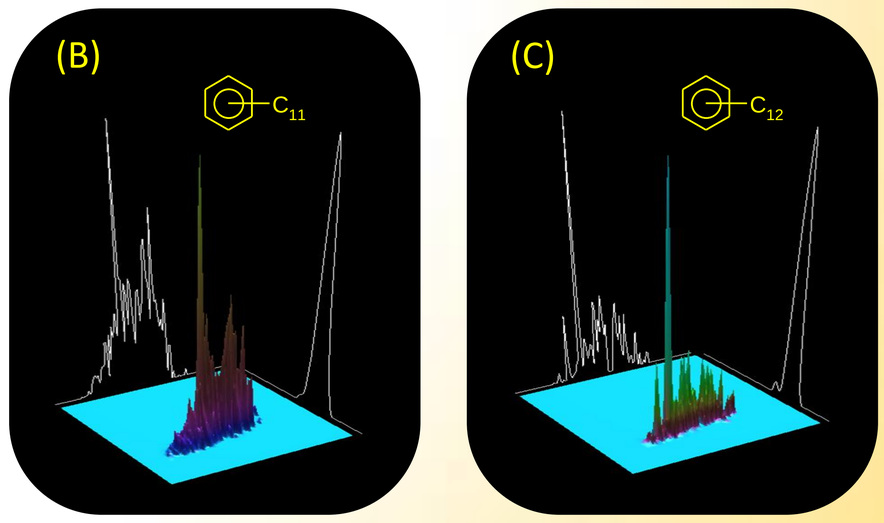


Figure 3. (A) Example extracted ion mass chromatogram (*m/z* 133+119+105) showing the chromatographic separation of C_3 to C_{12} branched alkyl benzene isomers. **(B)** Chromatographic separation of individual C_{11} (*m/z* 232) branched alkyl benzene isomers. **(C)** Chromatographic separation of individual C_{12} (*m/z* 246) branched alkyl benzene isomers.



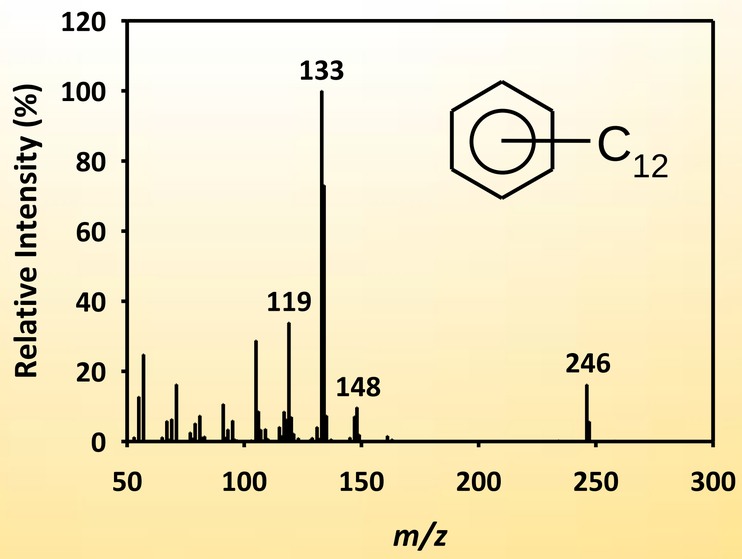


Figure 4. Example mass spectrum of a C_{12} branched alkyl benzene (BAB).

BABs have been reported to be toxic:

•Booth *et al*. (2007) Environmental Science & Technology 41, 457-464.

•Scarlett *et al*. (2008) Environmental Toxicology & Chemistry 27, 561-567.

•Scarlett *et al*. (2009) Environmental Toxicology & Chemistry 28, 381-387.

Conclusions

- The use of GCxGC-ToF-MS in the present study demonstrates improved chromatographic resolution of oil contaminated soil samples and when coupled to ToF-MS yields more reliable peak assignments from mass spectra than possible with conventional methods, thereby allowing vastly increased numbers of individual chemical components to be characterised.

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