Environmental Forensics: Employing 2-Dimensional Gas Chromatography/Mass Spectrometry (GCxGC/MS) to Predict Environmental Weathering of Oil and Tar

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I. Introduction

Pollution from petroleum sources and coal tar is the result of naturally occurring and unintended seepages; collection, transport, storage, and disposal. This pollution has significant impacts on human health and the environment. To address the weathering of these pollutants, a new approach using GCxGC/MS was developed to predict the environmental weathering of oil and tar.

II. Technology

Comprehensive GC/MS, GCxGC/MS, is a leading-edge separation technique. All of the effluent from the first-dimension column is focused in many narrow fractions at regular intervals and subsequently injected onto a second capillary column.

A new ion Analytics™ software visualizes extracted ion abundances as a histogram and normalizes them to the expected ion ratio of the target compound. Compound identity confirmation is automatically achieved according to spectral deconvolution algorithms that subtract background noise and match sample with library spectra.

The combination of spectral deconvolution software with modern fast-scanning quadrupole mass spectrometers has allowed the first quantification of pollutants by GCxGC/MS. A minimum of three modulations-per-compound and five scans-per-modulation was found to produce results in agreement with GC/MS analysis of parent PAH within 20% RPD, however sensitivity was increased 5- to 10-fold and GCxGC/MS provided much higher resolution.

III. Weather Maps

Understanding the impact that weathering processes have on hydrocarbon contamination is essential in risk assessment, forensic analyses and liability studies. GCxGC/MS offers the ability to visualize dissolution and evaporation processes based on retention characteristics on compounds on the 2D chromatogram.

Weathering effects were estimated via LFER based on compound's aqueous solubility (S_w), octanol-water partition coefficient (K_{ow}), and vapor pressure (V_v). These physical properties were linked to a compound's retention index, allowing component maps to be drawn that predict the progression of weathering based on site conditions (e.g. arid climate vs. high soil water content).

The figures depict changes in volatility and solubility for the sample as it undergoes weathering.

GCxGC/MS was used to create the 3D component maps for a "fresh" coal tar, collected from an underground storage tank protected from the environment and from soil contaminated with coal tar outside of the tank. The figures depict changes in volatility and solubility for the sample as it undergoes weathering.

References