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Characterisation of dense non-aqueous phase liquids of coal tar using comprehensive two-dimensional gas chromatography coupled with time of flight mass spectrometry.

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Comprehensive two-dimensional gas chromatography (GCxGC) is a recently developed analytical technique in which two capillary columns with different stationary phases are placed in series enabling planar resolution of the analytes. The resolution power of GCxGC is one order of magnitude higher than that of one dimension gas chromatography. Because of its high resolution capacity, the use of GCxGC for complex environmental samples such as crude oils, petroleum derivatives and polychlorinated biphenyls mixtures has rapidly grown in recent years. We developed a one-step method for the forensic analysis of coal tar dense non-aqueous phase liquids (DNAPLs) from former manufactured gas plant (FMGP) sites.

Coal tar is the by-product of the gasification of coal for heating and lighting and it is composed of thousands of organic and inorganic compounds. Before the boom of natural gases and oils, most towns and cities had one or several manufactured gas plants that have, in many cases, left a devastating environmental print due to coal tar contamination. The fate of coal tar DNAPLs, which can persist in the environment for more than a hundred years, is therefore of crucial interest.

The presented analytical method consists of a unique clean-up/ extraction stage by pressurized liquid extraction and a single analysis of its organic chemical composition using GCxGC coupled with time of flight mass spectrometry (TOFMS). The chemical fingerprinting is further improved by derivatisation by N,O-bis(trimethylsilyl)trifluoroacetamide (BSTFA) of the tar compounds containing –OH functions such as alcohols and carboxylic acids.

We present here how, using the logical order of elution in GCxGC-TOFMS system, 1) the identification of never before observed –OH containing compounds is possible and 2) the isomeric selectivity of an oxidation reaction on a DNAPL sample can be revealed.

Using samples collected at various FMGP sites, we demonstrate how this GCxGC method enables the simultaneous uncovering of information on the source of the coal tar, particularly the coal gasification process it originates from, and on its fate once released in the subsurface, i.e. the nature of the transformations it underwent such as evaporation, water-washing, chemical reactions or biodegradation.