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Parameter Optimisation for the Determination of Total Petroleum Hydrocarbons (Hydrocarbon Index) by Gas Chromatography Using the Large Volume Injection Technique

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Abstract — The determination of total petroleum hydrocarbons (hydrocarbon index) in water and soil is an important analytical task to assess levels of environmental pollution. The formerly common IR-absorption based method has recently been replaced by a gas chromatographic (GC) method that, however, lacks sufficient sensitivity. In order to reach the detection limits stipulated by environmental legislation, large volume injection (LVI) may be used for gas chromatography. Programmed-temperature vaporiser (PTV) injection can help to avoid the loss of volatile analytes and may be applied instead of a preconcentration procedure. The optimisation of the experimental parameters of PTV LVI for determination of petroleum hydrocarbons is discussed in this contribution.

I. INTRODUCTION

Water pollution by petroleum hydrocarbons is an important environmental problem. The determination of total petroleum hydrocarbons (hydrocarbon index) in water and soil is complicated by the fact that total petroleum hydrocarbons (TPH) are a large group of compounds including as different mixtures as crude oil and refined petroleum products. Currently, there are two standard methodologies based on GC as substitutes for the former IR method that was abandoned due to the use of chlorofluorocarbons in the extraction, which can be used to monitor the maximum hydrocarbon content.

- ISO 9377-2: 2000 – the official European standard method for the determination of hydrocarbon oil index in water by GC-FID;

Both methods are based on extraction of water samples with a nonpolar (hydrocarbon) solvent, capillary GC measurement, and determination of the total peak area of compounds eluting between n-decane (C10H22) and n-tetracontane (C40H82) for the ISO 9377-2 standard. The OSPAR method was modified to include the determination of certain hydrocarbons with boiling point starting already from 98°C (from n-heptane) with particular consideration of the TEX (toluene, ethylbenzene and o-/p-/m-xylene) compounds.

To reach the required detection limit, the method according to ISO 9377-2:2000 foresees preconcentration of the extracts by solvent evaporation. In contrast to this, the OSPAR method does not allow for any external apparatus for preconcentration, for which reason the GC must be equipped with an injection system that allows the injection of up to 50 µl of the extract. Typically, programmed-temperature vaporiser large volume injectors (PTV LVI) are used for this reason.

PTV injection separates solvent vapour from analytes through venting of the vapour in the liner. The PTV large volume injector is equipped with a very sophisticated temperature, flow and pressure control and speed-controlled injections functions.

Optimisation of the PTV LVI method involves the correct adjustment of:

- Injector initial temperature
- Solvent evaporating temperature program
- Injection rate, injected amount
- Solvent split rate and time
- Purge vent rate and time
- Inlet pressure

Problems such as sample discrimination, partial or complete loss of early eluting peaks, peak deformation (splitting) and carry over can occur in PTV LVI if the above mentioned parameters are not carefully optimized.
II. EXPERIMENTAL

The work was carried out using an Agilent 7890A GC system, equipped with a UNIS 2100 large volume injector, a flame ionisation detector (FID) operated at 340 °C and with a CombiPal CTC autosampler allowing PTV-large volume injection. Instrument control and data evaluation was done with the ChemStation software. GC Oven program: 35 °C (6 min), with 35 °C/min to 340 °C (6 min). The optimised parameters for programmed-temperature vaporiser large volume injector are:

PTV program: -20 °C (0 min), 720 °C/min to 340 °C (15 min). Solvent vent flow: 100 ml/min; Solvent vent time: 0 min; Vent pressure: 10 psi; Purge flow: 100 ml/min; Purge time: 1 min; Injection volume: 50 µl; Injection speed: 5 µl/sec.

A UNIS straight liner with a length of 88 mm and 3 mm ID, packed with deactivated borosilicate glass wool was used. A Restek RTX-5MS 30 m x 0.25 mm ID, 0.25 µm capillary column with an uncoated 5 m x 0.32 mm ID, deactivated fused silica capillary as precolumn (Supelco) were used.

A standard mixture, consisting of C7, C10, C20, C40 and TEX compounds in pentane, at 5 µg/ml each, was used to test the analytical performance of the method and system. The recovery of the components was determined experimentally. Normalized peak areas were used for calculation of component recoveries. The relative response (peak area, PA) of n-decane (C10) and n-tetracontane (C40) compared with n-eicosane (C20) was investigated.

III. RESULTS AND DISCUSSION

When injecting larger volumes, the removal of the largest part of the solvent is necessary in order to concentrate the analytes and maintain good separation. The sample introduction rate must thus be equal to or slightly higher than its evaporation rate.

The injection speed can be estimated using the equation (1) for solvent elimination rate [v, µl/min] calculation:

\[
v = \frac{M \times P_v}{\rho \times R \times T_{inlet}} \times \frac{P_a}{P_{inlet}} \times V_{sf}
\]

where:
- \(M\) – molecular weight of solvent [g/mol]
- \(P_v\) – vapour press. of solv. at initial inlet temp. [bar]
- \(\rho\) – density of solvent [g/ml]
- \(R\) – gas constant [0.08312 l*bar/K*mol]
- \(T_{inlet}\) – initial temperature of inlet [K]
- \(P_a\) – ambient pressure [usually 1.013 bar]
- \(P_{inlet}\) – inlet pressure [gauge+ambient pressure, bar]
- \(V_{sf}\) – split flow [ml/min]

Equation (1) reveals how the LVI parameters are interrelated and need to be optimised. This has been done for the determination of TPH, where a chromatogram obtained under the optimised conditions is shown in Figure 1.

![GC chromatogram of 50 µl injection of system performance test performed at the optimised parameters](image)

Figure 1: GC chromatogram of 50 µl injection of system performance test performed at the optimised parameters

Figure 2 reports recoveries for the components of the standard mixture under conditions deviating from the optimum set of parameters for PTV LVI.

![Comparison of relative response between C7, C10, C20 and C40](image)

Figure 2: Comparison of relative response between C7, C10, C20 and C40,

IV. CONCLUSION

We have demonstrated the importance of parameter optimisation for GC with LVI for TPH analysis. In addition to the parameter addressed in this study, other factors such as liner design and packing are important and need to be investigated.

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