THE SCIENCE OF ACQUITY UPLC APPLIED TO ENVIRONMENTAL ANALYSES OF PAHs AND EXPLOSIVES IN WATER

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INTRODUCTION

Polynuclear Aromatic Hydrocarbons (PAHs) and explosive residues are ubiquitous contaminants in our environment; the former as a result of many industrial processes, the latter due to military activity. Standard and official methods for the analysis of PAHs and explosives are found in compendia for air, water, solid waste and food analysis[1]. These methods specify HPLC with run times in excess of 30 minutes. The Waters® ACQUITY UltraPerformance LC® (UPLC®) system can perform these same analyses in less than 10 minutes, a reduction of over 60 percent. Additionally, the lower flow rates of the ACQUITY UPLC system decrease the amounts of solvent consumed and waste generated, providing a cost savings for the laboratory.

APPLICATIONS

Polynuclear aromatic hydrocarbons

The analysis of PAHs is a high priority environmental application. Using HPLC, injection-to-injection cycle times exceeding 45 minutes are common, resulting in the completion of only 10 to 11 analyses over the course of a typical eight-hour working shift. Figure 1 illustrates the UPLC separation of 21 PAH analytes with a run time of only 7 minutes. The shorter run time allows for the analysis of over 50 samples in the same eight-hour shift. Higher sensitivity and superior peak shape result in more accurate quantitation.

Explosives residues

Explosives residues in soil or water are of both forensic and environmental concern. Military sites around the world have produced, stockpiled, expended and disposed of explosives for many years. These munitions contain nitroaromatic and nitramine compounds, which can pose a significant human health risk.

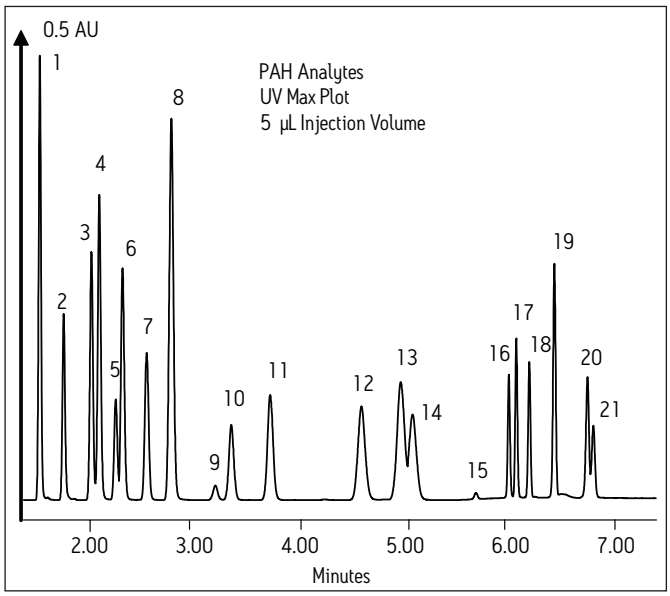

Figure 1. PAH analysis using an ACQUITY UPLC column, 2.1 x 100 mm, 1.7 micron BEH C18. A water:acetonitrile gradient from 66 to 90% acetonitrile at a flow rate of 0.4 mL/min was used. Detection was UV Maxplot mode. Sample was a 5 µL injection. 10 parts per million (ppm) analyte mixture as follows:

1: *Naphthalene*
2: *Acenaphthalene*
3: *1- Methylnaphthalene*
4: *2-methyl-naphthalene*
5: *Fluorene*
6: *Acenaphthene*
7: *Phenanthrene*
8: *Anthracene*
9: *Decafluorobiphenyl*
10: *Fluoranthene*
11: *Pyrene*
12: *p-Terphenal-d-14*
13: *Chrysene*
14: *Benzo(a)anthracene*
15: *Decachlorobiphenyl*
16: *Benzo(b)fluoranthene*
17: *Benzo(k)fluoranthene*
18: *Benzo(a)pyrene*
19: *Dibenzo(a,h)anthracene*
20: *Indeno(1,2,3-cd)pyrene*
21: *Benzo(g,h,i)perylene.*

HPLC-based assays of these compounds have proven to be challenging due to the selectivity needed to resolve positional isomers. In addition, HPLC methods (e.g. IPA in water) require viscous buffered mobile phases operated at high temperatures (40 °C) and analysis times exceeding 30 minutes.[2]

Figure 2 shows the separation of a complex mixture of explosive compounds and its degradates using the ACQUITY UPLC system. The analysis is completed in less than 7 minutes with a much simpler, more robust water:methanol mobile phase.

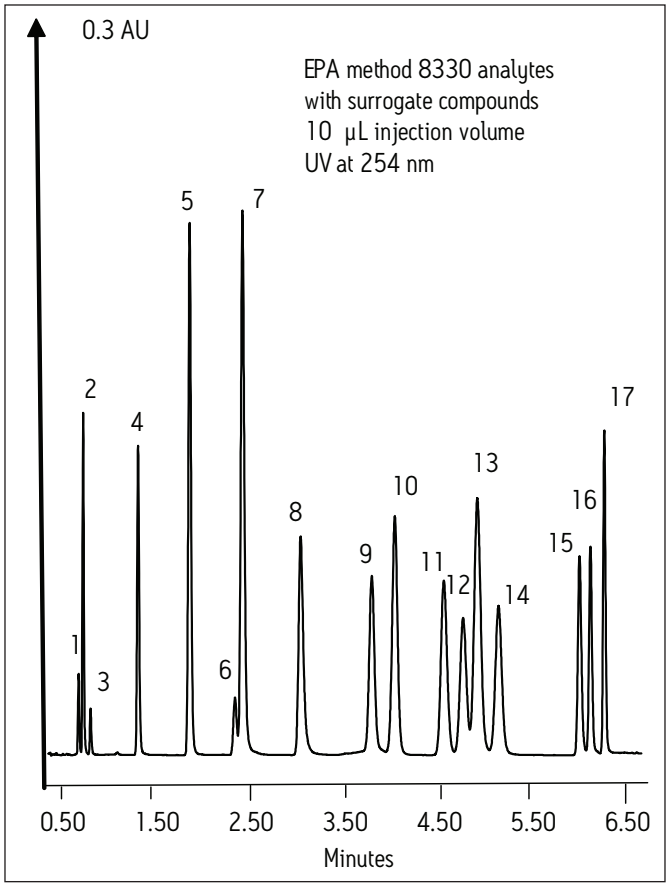

Figure 2. Explosives analysis using the ACQUITY UPLC column, 2.1 x 100 mm, 1.7 micron BEH C_{18}. A water:methanol gradient from 31 to 60% methanol at a flow rate of 0.5 mL/min was used. Detection was UV @ 254 nm. Sample was a 5 µL injection 10 ppm analyte mixture as follows:

*1: 2,6 Diamino - 4 nitrotoluene**
2: HMX
*3: 2,4 Diamino - 6 nitrotoluene**
4: RDX
5: 1,3,5 - Trinitrotoluene
*6: 1,2 - Dinitrobenzene**
7: 1,3 - Dinitrobenzene
8: Nitrobenzene
9: Tetryl
10: 2,4,6 - Trinitrotoluene
11: 2 - Amino - 4,6 - Dinitrotoluene
12: 4 - Amino - 2,6 - Dinitrotoluene
13: 2,4 - Dinitrotoluene
14: 2,6 - Dinitrotoluene
15: 2 - Nitrotoluene
16: 4 - Nitrotoluene
17: 3 - Nitrotoluene

** Surrogate compounds.*

CONCLUSION

The ACQUITY UPLC system significantly decreases run times while improving selectivity and sensitivity in the analysis of PAHs and explosives. At a time when scientists have reached barriers pushing the limits of conventional HPLC, UPLC provides the technology to extend and expand the utility of separation sciences.

References

1. AOAC 973.30; Deutsche DIN TVO; UK ISBN 0 11 & 752032 2; U.S EPA Methods TO-13, 550 & 550.1, 610, 8310 & 8330.
2. Oasis® Applications Notebook, page 82, Waters Corporation.

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