「Application Note」

PAHs (Polycyclic Aromatic Hydrocarbons) Analysis by GC/MS with EPA 8270E

- GC/MS Application

Abstract

PAHs (Polycyclic aromatic hydrocarbons) are organic chemicals that are composed of a group of multiple benzene rings having many types of isomers. Some kinds of PAHs are known as toxic or cancer-causing compounds and there are 17 kinds of priority PAHs identified by US EPA (Environmental Protection Agency) and 33 kinds of prioty PAHs by WHO (World Health Organization). PAHs are exposed to human in natural source such as volcanic eruptions, crude oils or forest fires and manmade combustion source such as industrial process, fossil fuels or vehicles, etc. Low molecular weight PAHs can be biologically degradated but most of PAHs are generally insoluble in water. The more benzene rings PAHs have, the lower volatility they feature and this produces dusts absorbed with PAHs or residuals compounds on soils or sediments. This study shows the analysis of PAHs in surface water by YL6900 GC/MS with EPA 8270E (Semivolatile Organic Compounds By Gas Chromatography/Mass Spectrometry).

Instruments and Software

· YL6900 GC/MS System

Item	Description	Part No.
Oven	6500 GC Oven System Module	6501011012
Inlet	Capillary inlet system for 6500 GC	6501011023
Detector	YL6900 MS for YL6500 GC incl. built-in turbomolecular pump - Single Quadrople - EI source - Turbo pump(240 L/sec) - Include fore pump and spares kit	6501011440
Install. Option	Start-up kit includes (Without GC Capillary Column) 1) Nuts and ferrules 1/8" 2) Nuts, 1/4" 3) Vespel ferrule, 1/4" 4) Union Tee, 1/8" 5) Septa, 11 mm, 50/pk 6) Tubing cutter 7) Monkey spanner 8) Wrench 1/2" & 9/16" 9) Wrench 1/2" & 7/16" 10) Wrench 3/8" & 7/16" 11) Wrench 1/4" & 5/16" 12) (+) screw driver 6x100 13) (+) screw driver 5x100 14) (-) screw driver 6x100 15) Leak detection fluid 16) 10 µL syringe 17) Copper tubing, 1/8"	1601011110
YL Liquid Autosampler	YL3000A Autosampler for GC. 121 positions tray for 2 mL vials. Includes 10 µL syringe Right Hand Mount	6501432540
	Installation kit for YL3000 series Autosampler to YL6500 GC	6501011240
CDS	YL-Clarity software for single instrument of YL GC	5301011020
	MS module of YL-Clarity(Library 별도)	5301011180
	Autosampler control of YL-Clarity	5301011040
	Library(NIST/EPA/NIH 2017 edition)-306,622 spectra	NIST17-MS-LIB
Column	YL 5ms (30m x 0.25mm i.d. x 0.25um)	1256120170
ACC	Autosampler vial 100/pk	21154
	Autosampler vial cap, PTFE/silicone septa 100/pk	24485

Reagents and Standards

Polynuclear aromatic hydrocarbons 18 mix (2000 µg/mL each component in benzene : dichloromethane = 50:50)

Preparation of Standard Solution

Polynuclear aromatic hydrocarbons mix standard 20.0 mg/L was diluted to 0.050 mg/L, 0.100 mg/L, 0.250 mg/L, 0.500 mg/L, 1.000 mg/L by Dichloromethane to make a calibration curve.

The sample of 1,000 mL was spiked at concetrations as follows. (0.050 µg /L, 0.100 µg /L, 0.250 µg /L, 0.500 µg /L, 1.000 µg /L)

Fig 1. YL6900 GC/MS

Preparation of Water Samples

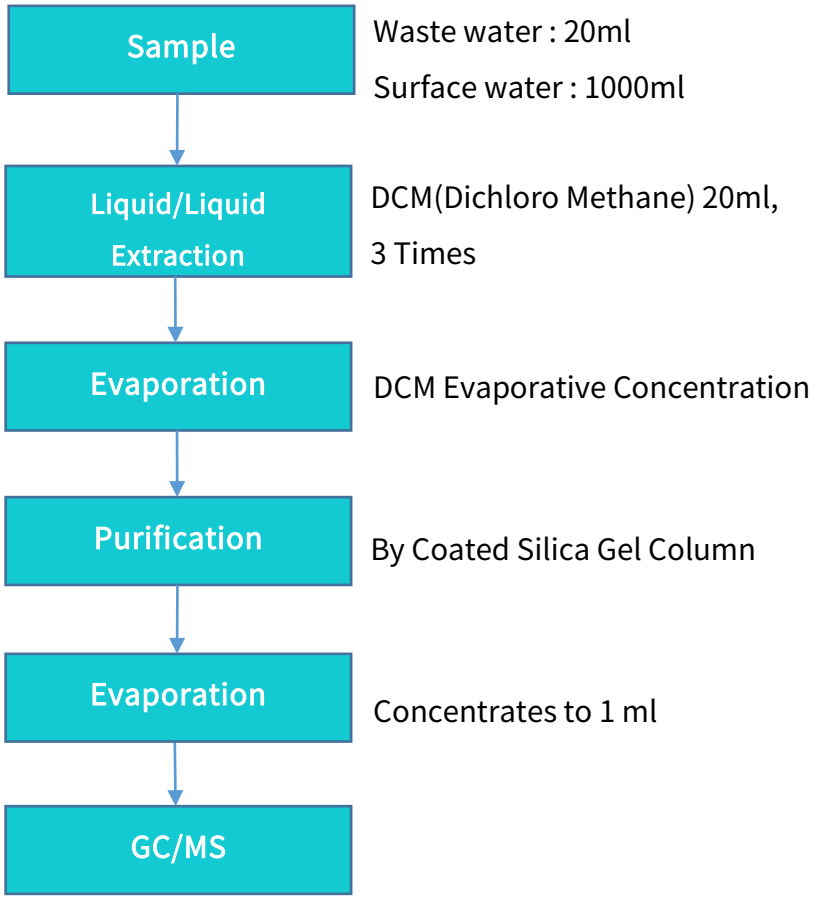

Table 1. Preparation of Water

For water sample preparation, the volume of sample varies depending on sample matrix following to the steps indicated in Table 1. Add DCM to the water sample and wait for layers forming by Liquid/Liquid Extraction. Then, mixing with Sodium Sulfate, DCM will be lost during the contration step. After repeating this step 3 times, there will be 60 ml of DCM collected and this is to be evaporated by nitrogen upto 1ml. The concentrated sample The purifiacation by Silica Gel Column is necessary and the purified sample needs to be concentrated up to 1 ml. The collected sample is placed into GC vials for analysis.

Table 2 shows GC/MS analysis conditions and PAHs are analyzed in SIM mode.

GC conditions	MS conditions
Column: YL 5ms (30m x 0.25mm I.D. x 0.25µm)	Ion source 250°C, Transfer Line 280°C
Inlet: split, 1/10 split ratio, 1µl Injection	Detection: SIM mode
Oven temperature program : 70°C, 5min, 8°C/min to 300°C, 10min	

Table 2. GC/MS Condition

	Compound	Formula	Molecular Weight	Selected Ions, m/z
1	Naphthalene	C10H8	128.17	128
2	2-Methylnaphthalene	C11H10	142.20	142
3	1-Methylnaphthalene	C11H10	142.20	142
4	Acenaphthylene	C12H8	152.19	152
5	Acenaphthene	C12H16	154.21	154
6	Fluorene	C13H10	166.22	166
7	Phenanthrene	C14H10	178.23	178
8	Anthracene	C14H10	178.23	178
9	Fluoranthene	C16H10	202.25	202
10	Pyrene	C16H10	202.25	202
11	Benzo(a)anthracene	C18H12	228.29	228
12	Chrysene	C18H12	228.29	228
13	Benzo(b)fluoranthene	C20H12	252.31	252
14	Benzo(k)fluoranthene	C20H12	252.31	252
15	Benzo(a)pyrene	C20H12	252.31	252
16	Indeno(1, 2, 3-cd)pyrene	C22H12	276.33	276
17	Dibenzo(a, h)anthracene	C22H14	278.35	278
18	Benzo(g, h, i)perylene	C22H12	276.33	276

Table 3. GC/MS Chromatographic Conditions for 18 PAHs

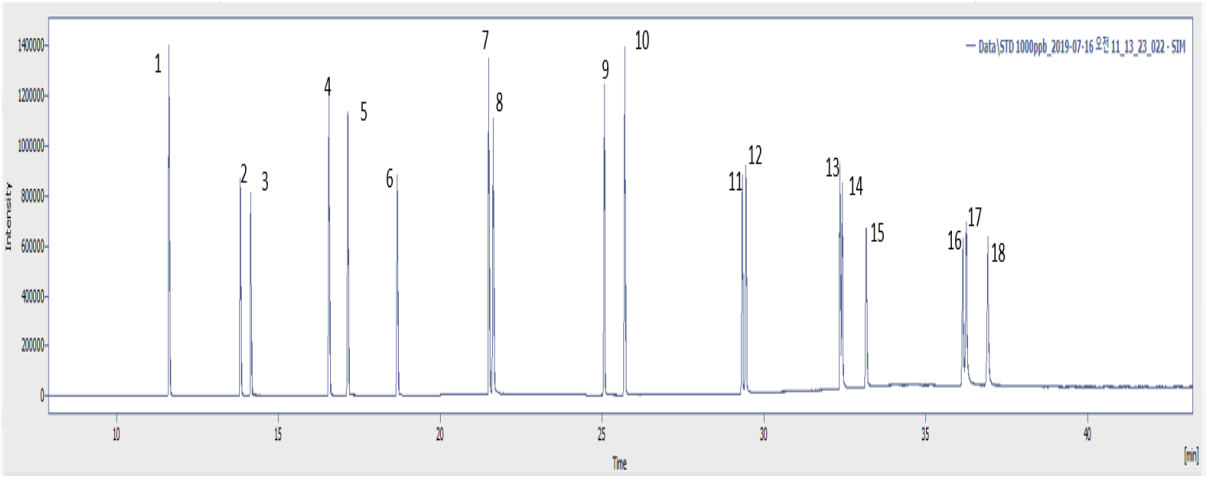

Fig 2. PAHs Chromatogram [1. Naphthalene, 2. 2-Methylnaphthalene, 3. 1-Methylnaphthalene, 4. Acenaphthylene, 5. Acenaphthene, 6. Fluorene, 7. Phenanthrene, 8. Anthracene, 9. Fluoranthene, 10. Pyrene, 11. Benzo(a)anthracene, 12. Chrysene, 13. Benzo(b)fluoranthene, 14. Benzo(k)fluoranthene, 15. Benzo(a)pyrene, 16. Indeno(1, 2, 3-cd)pyrene, 17. Dibenzo(a, h)anthracene, 18. Benzo(g, h, i)perylene]

	Analyte	R.T(min)	MDL(μg /L)	Accuracy (%)	Precision
1	Naphthalene	11.617	0.022	103.93	2.00
2	2-Methylnaphthalene	13.820	0.013	99.79	2.86
3	1-Methylnaphthalene	14.143	0.009	94.97	4.27
4	Acenaphthylene	16.560	0.020	107.97	5.69
5	Acenaphthene	17.137	0.016	107.97	5.69
6	Fluorene	18.667	0.008	108.39	4.89
7	Phenanthrene	21.497	0.013	99.68	6.93
8	Anthracene	21.633	0.031	99.73	5.15
9	Fluoranthene	25.063	0.021	104.38	6.01
10	Pyrene	25.697	0.008	104.49	3.93
11	Benzo(a)anthracene	29.323	0.016	104.92	1.57
12	Chrysene	29.437	0.025	98.04	1.83
13	Benzo(b)fluoranthene	32.350	0.024	95.92	6.32
14	Benzo(k)fluoranthene	32.413	0.026	101.35	3.33
15	Benzo(a)pyrene	33.157	0.014	101.85	2.31
16	Indeno(1, 2, 3-cd)pyrene	36.140	0.007	100.32	0.43
17	Dibenzo(a, h)anthracene	36.250	0.027	100.16	7.30
18	Benzo(g, h, i)perylene	36.907	0.011	100.39	2.04

Table 4. Validity of Test Method

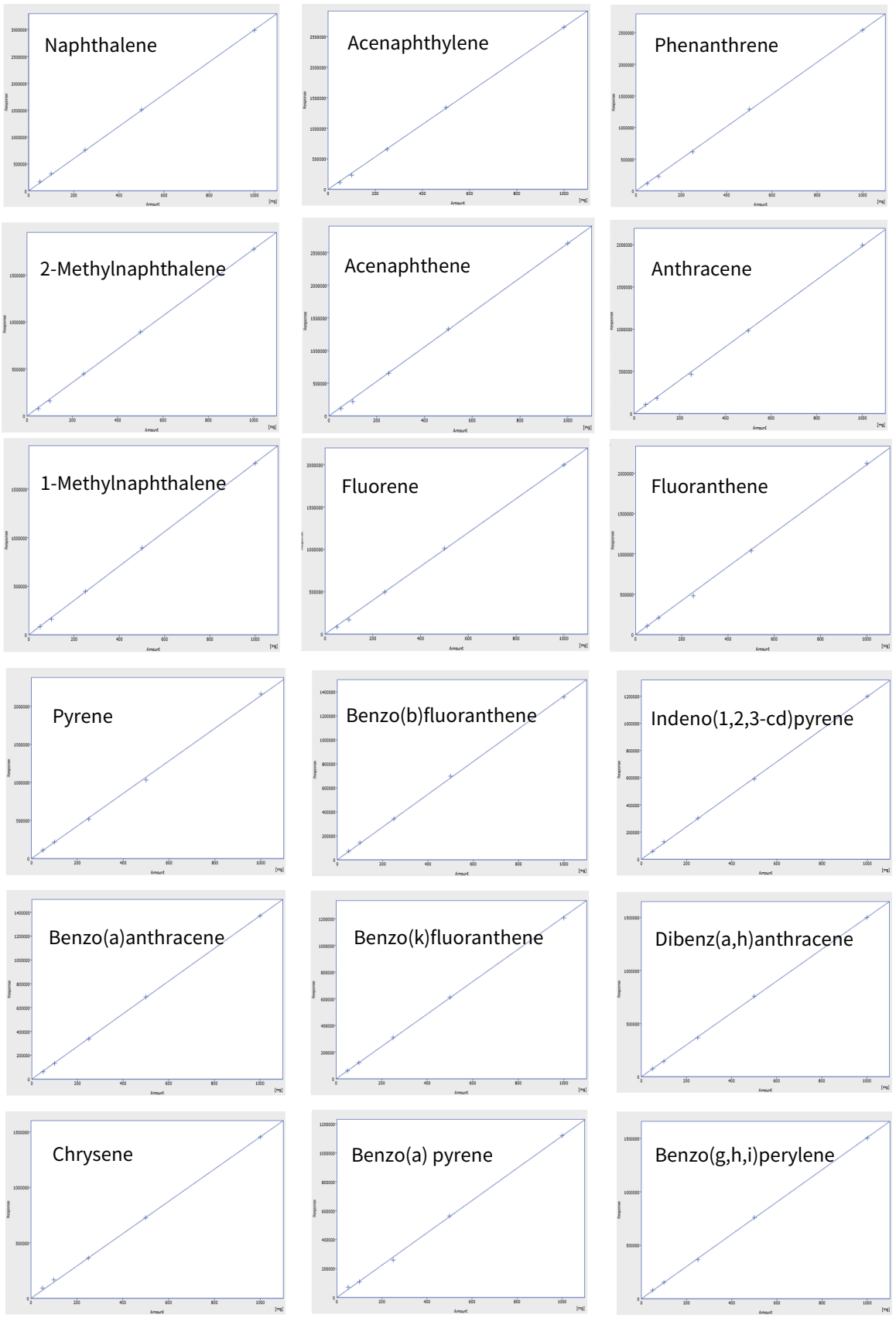

Fig 3. Verification of Calibration Curve

Result

To determine the validity of test results, linearity, accuracy, precision (RSD %) and method detection limit (MDL) were generated and the the calibration curve R^2 value of each compounds in PAHs by the 5-point of concentrations indicated on [Fig 2] & [Table 4] is over 0.999. [Fig 3]

This result refered to ' Environmental Research & Test QA/QC Handbook' by Korean National Institute of Environmental Research.

The surface water was spiked with 0.250 mg/L of standard reference and % recovery meets between 90~110 %. [Fig 4] [Table 5]

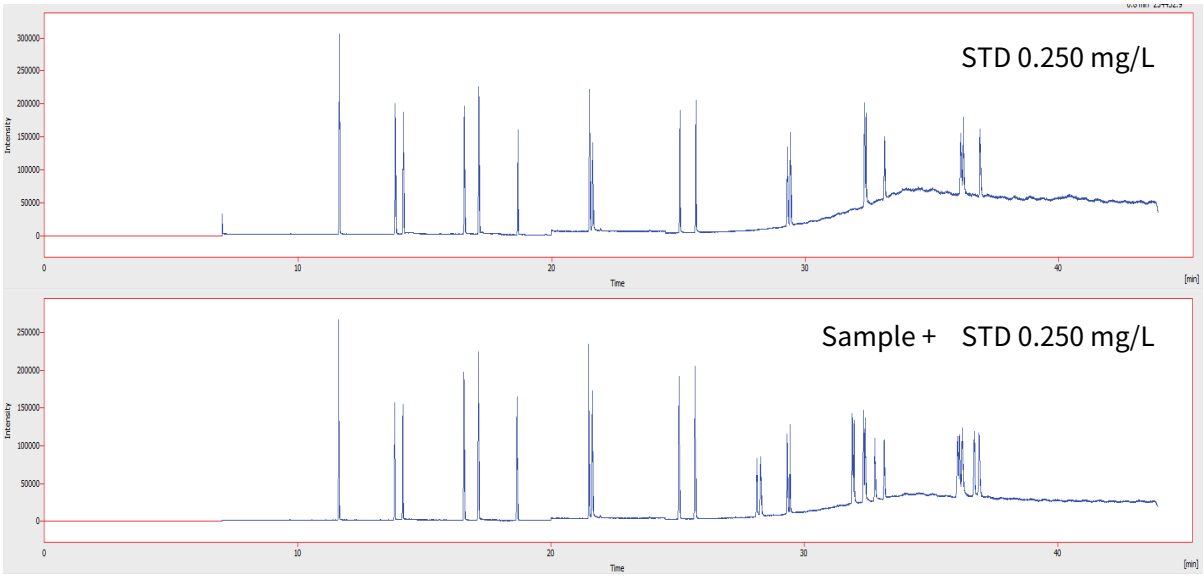

Fig 4. Sample Chromatogram (STD 0.025 mg/L spiking)

	Analyte	Recovery (%)		Analyte	Recovery (%)
1	Naphthalene	90	10	Pyrene	101
2	2-Methylnaphthalene	91	11	Benzo(a)anthracene	90
3	1-Methylnaphthalene	94	12	Chrysene	94
4	Acenaphthylene	103	13	Benzo(b)fluoranthene	91
5	Acenaphthene	101	14	Benzo(k)fluoranthene	91
6	Fluorene	100	15	Benzo(a)pyrene	90
7	Phenanthrene	109	16	Indeno(1, 2, 3-cd)pyrene	91
8	Anthracene	107	17	Dibenzo(a, h)anthracene	92
9	Fluoranthene	99	18	Benzo(g, h, i)perylene	92

Table 5. Sample Recovery

Conclusion

In this study, 18 kinds of PAHs in water were analyzed by YL6500 GC/MS and YL6500 GC/MS verifies reliable data in accordance with EPA 8270E.

Reference

- EPA Method 8270E (Semivolatile Organic Compounds By Gas Chromatography /Mass Spectrometry)

- Environmental Research & Test QA/QC Handbook by Korean National Institute of Environmental Research (2011)

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