

Supporting information

Field performance of the Chemcatcher passive sampler for monitoring hydrophobic organic pollutants in surface water

Branislav Vrana*^a, Graham A. Mills^b, Pim E. G. Leonards^c, Michiel Kotterman^d, Mona Weideborg^e, Jana Hajšlová^f, Vladimír Kocourek^f, Monika Tomaniová^f, Jana Pulkrabová^f, Marie Suchanová^f, Kateřina Hájková^f, Sirpa Herve^g, Heidi Ahkola^g and Richard Greenwood^h

^a*Slovak National Water Reference Laboratory, Water Research Institute, Nabr. arm. gen. L. Svobodu 5, 81249 Bratislava, Slovakia. Fax: ++421 2 544 18047; Tel: ++421 2 593 43 466; E-mail: branovrana@googlemail.com*

^b*School of Pharmacy and Biomedical Sciences, University of Portsmouth, White Swan Road, PO1 2DT, UK*

^c*Institute for Environmental Studies (IVM) VU University Amsterdam, De Boelelaan 1087,1081 HV Amsterdam, The Netherlands*

^d*Netherlands Institute for Fisheries Research (RIVO), P.O. Box 68, 1970 AB IJmuiden, The Netherlands*

^e*Aquateam AS, Hasleveien 10, 0571 Oslo, Norway*

^f*Institute of Chemical Technology, Technická 5, 16628 Prague, Czech Republic*

^g*Finnish Environment Institute, P.O. Box 110, Jyväskylä FIN-40101, Finland*

^h*School of Biological Sciences, University of Portsmouth, King Henry I Street, Portsmouth, PO1 2DY, UK*

Table SI - 1. Selected physicochemical properties of test analytes.

Compound	MW^a	log <i>K</i>_{ow}^b	S^c
	[g mol⁻¹]		[g m⁻³]
Biphenyl	154.2	3.8	7.48
Acenaphthene	154.2	4.0	3.80
Fluorene	166.2	4.2	1.90
Anthracene	178.2	4.6	0.045
Phenanthrene	178.2	4.5	1.100
Fluoranthene	202.3	5.1	0.260
Pyrene	202.3	5.1	0.132
Benzo[a]anthracene	228.3	5.9	0.011
Chrysene	228.3	5.7	0.0019
Benzo[b]fluoranthene	252.3	5.8	0.0015
Benzo[k]fluoranthene	252.3	6.0	0.0008
Benzo[a]pyrene	252.3	6.2	0.0038
Indeno[1,2,3cd]pyrene	276.3	6.8	0.0005
Dibenz[a,h]anthracene	278.4	6.8	0.0024
Benzo[g,h,i]perylene	276.3	6.9	0.0003
Pentachlorobenzene	250.3	5.2	0.831
Hexachlorobenzene	284.8	5.5	0.005
Lindane	290.8	3.7	7.3
Endosulfan I	406.9	3.8	0.51
Dieldrin	380.9	5.4	0.195

^aMolecular weight (MW); ^boctanol/water partition coefficient (*K*_{ow}); ^caqueous solubility at 25°C (*S*)

Recovery of analytes from passive samplers

Accuracy was evaluated on the basis of analyte recovery from spiked Chemcatchers prepared by University of Portsmouth. Before the start of the field trial, each of the 4 partners performing the field trial, received a set of 3 Chemcatchers spiked with 1 μg of each target analyte. Percent recovery was determined by:

$$\% \text{Recovery} = (\text{measured analyte concentration} / \text{spike concentration}) \times 100$$

Table SI-2 Mean and range of percent recoveries of target analytes from spiked Chemcatcher samplers, n = 12.

Compound	MEAN	RANGE
	Spike recovery (%)	Spike recovery (%)
Acenaphthene	87	69-115
Fluorene	61	6-84
Phenanthrene	90	79-109
Anthracene	73	57-98
Fluoranthene	94	74-122
Pyrene	95	81-127
Benz[a]anthracene	98	73-131
Chrysene	47	42-54
Benzo(b)fluoranthene	100	68-144
Benzo(k)fluoranthene	64	52-79
Benzo(a)pyrene	65	40-87
Indeno[1,2,3-cd]pyrene	67	41-98
Dibenz[a,h]anthracene	54	31-80
Benzo[g,h,i]perylene	50	33-67
Benzene, pentachloro-	86	74-100
Benzene, hexachloro-	78	51-93
Lindane	104	92-121

Concentration of analytes found in fabrication controls

24 fabrication control samplers were analysed for contaminant content during the field trial. Quantifiable concentrations of 7 PAHs were determined in the fabrication blanks (Fig. SI-3). Phenanthrene was the fabrication blank contaminant present at highest concentrations, up to 90 ng/ sampler. The high variation of the levels found in fabrication blanks indicates that the contamination occurred not only during the sampler preparation, but also during their subsequent shipment, handling and extraction.

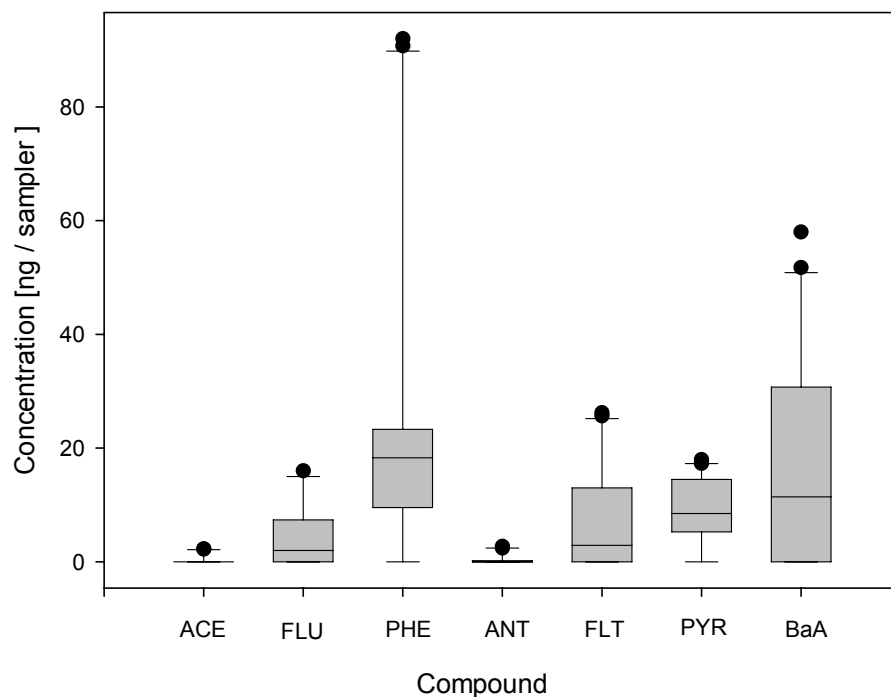


Figure SI-1. A box plot showing concentrations of target analytes determined in all fabrication controls analysed during the field trial (n = 24). Compounds not shown in the graph were not detected in control samplers. The boundary of the box closest to zero indicates the 25th percentile, a line within the box marks the median, and the boundary box farthest from zero indicates the 75th percentile. Error bars above and below the box indicate 90th and 10th percentiles. The black dots indicate outlying points.

Table SI-3. Exchange rate constants k_e of performance reference compounds estimated using Equation 2 from the PRC levels found in the fabrication blanks (m_{D0}) and samplers exposed at three sampling sites in Europe. Values are reported only in case the corresponding k_e value was statistically significant.

k_e [d^{-1}], 14 days exposure, Spring 2004					
Sampling site	D-BIP^a	D-ACE^b	D-FLU^c	D-PHE^d	D-PYR^e
Alna	0.020	0.014	0.010	0.005	
Meuse	0.046	0.036	0.027	0.014	
Elbe	0.062	0.040	0.036		
k_e [d^{-1}], 28 days exposure, Spring 2004					
Sampling site	D-BIP	D-ACE	D-FLU	D-PHE	D-PYR
Alna	0.012	0.010	0.007	0.003	
Meuse			0.021	0.012	
Elbe			0.030	0.013	
k_e [d^{-1}], 14 days exposure, Autumn 2004					
Sampling site	D-BIP	D-ACE	D-FLU	D-PHE	D-PYR
Alna	0.042	0.027	0.017	0.009	
Meuse	0.021	0.017	0.011		
Elbe	0.035	0.032			
k_e [d^{-1}], 28 days exposure, Autumn 2004					
Sampling site	D-BIP	D-ACE	D-FLU	D-PHE	D-PYR
Alna	0.029	0.020	0.013		
Meuse	0.018	0.014	0.009	0.004	
Elbe	0.032	0.027			

^aD-BIP = D₁₀-biphenyl

^bD-ACE = D₁₀-acenaphthene

^cD-FLU = D₁₀-fluorene

^dD-PHE = D₁₀-phenanthrene

^eD-PYR = D₁₀-pyrene

Table SI-4. Summary of in situ sampling rates (R_s) of determined for selected analytes during the spring field trials in three European rivers.

Compound	Log K_{ow}	Alna		Meuse		Elbe	
		14 days	28 days	14 days	28 days	14 days	28 days
Acenaphthene	4	0.044	0.029	0.117	0.081	0.159	0.101
Fluorene	4.2	0.075	0.050	0.199	0.137	0.270	0.171
Phenanthrene	4.5	0.113	0.075	0.298	0.206	0.406	0.256
Anthracene	4.6	0.118	0.078	0.312	0.216	0.424	0.268
Fluoranthene	5.1	0.087	0.058	0.23	0.159	0.313	0.198
Pyrene	5.1	0.087	0.058	0.23	0.159	0.313	0.198
Benz[a]anthracene	5.9	0.018	0.012	0.049	0.034	0.066	0.042
Chrysene	5.7	0.029	0.019	0.076	0.052	0.103	0.065
Benzo(b)fluoranthene	5.8	0.023	0.015	0.061	0.042	0.083	0.052
Benzo(k)fluoranthene	6	0.015	0.010	0.039	0.027	0.053	0.034
Benzo(a)pyrene	6.2	0.01	0.006	0.026	0.018	0.035	0.022
Indeno[1,2,3- cd]perylene	6.8	0.004	0.003	0.011	0.007	0.015	0.009
Dibenz[a,h]anthracene	6.8	0.004	0.003	0.011	0.007	0.015	0.009
Benzo[g,h,i]perylene	6.9	0.004	0.003	0.01	0.007	0.014	0.009
Pentachlorobenzene	5.2	0.079	0.052	0.208	0.144	0.283	0.179
Hexachlorobenzene	5.5	0.044	0.029	0.115	0.08	0.157	0.099
Lindane	3.7	0.013	0.008	0.034	0.023	0.046	0.029
Dieldrin	5.4	0.053	0.035	0.141	0.097	0.191	0.121

Table SI-5. Summary of in situ sampling rates (R_s) of determined for selected analytes during the autumn field trials in three European rivers.

Compound	LogK _{ow}	Alna		Meuse		Elbe	
		14 days	28 days	14 days	28 days	14 days	28 days
Acenaphthene	4	0.084	0.071	0.057	0.035	0.116	0.101
Fluorene	4.2	0.143	0.121	0.097	0.06	0.196	0.172
Phenanthrene	4.5	0.215	0.181	0.145	0.09	0.295	0.258
Anthracene	4.6	0.225	0.19	0.152	0.094	0.309	0.27
Fluoranthene	5.1	0.166	0.14	0.112	0.069	0.228	0.199
Pyrene	5.1	0.166	0.14	0.112	0.069	0.228	0.199
Benz[a]anthracene	5.9	0.035	0.03	0.024	0.015	0.048	0.042
Chrysene	5.7	0.054	0.046	0.037	0.023	0.075	0.065
Benzo(b)fluoranthene	5.8	0.044	0.037	0.03	0.018	0.06	0.052
Benzo(k)fluoranthene	6	0.028	0.024	0.019	0.012	0.039	0.034
Benzo(a)pyrene	6.2	0.019	0.016	0.013	0.008	0.025	0.022
Indeno[1,2,3-cd]pyrene	6.8	0.008	0.006	0.005	0.003	0.011	0.009
Dibenz[a,h]anthracene	6.8	0.008	0.006	0.005	0.003	0.011	0.009
Benzo[g,h,i]perylene	6.9	0.007	0.006	0.005	0.003	0.01	0.009
Pentachlorobenzene	5.2	0.15	0.127	0.101	0.063	0.206	0.18
Hexachlorobenzene	5.5	0.083	0.07	0.056	0.035	0.114	0.1
Lindane	3.7	0.024	0.021	0.016	0.01	0.033	0.029
Dieldrin	5.4	0.101	0.085	0.068	0.042	0.139	0.121

Table SI-6. TWA water concentrations calculated from spot samples and passive sampling data at the sampling site in the Meuse during the spring campaign (Trial I).

Compound	Spot samples 14 days	Spot samples 28 days	Chemcatcher 14 days	Chemcatcher 28 days
Acenaphthene	1.1	1.3	n.q.	n.q.
Fluorene	1.6	1.8	9.5	6
Phenanthrene	7.4	14.2	14	8
Anthracene	1.3	2.7	n.q.	n.q.
Fluoranthene	10.5	32.3	14.0	13.0
Pyrene	19.7	84.0	16.0	15.0
Benz[a]anthracene	5.5	7.0	n.q.	n.q.
Chrysene	8.8	10.1	5.0	6.0
Benzo(b)fluoranthene	2.6	3.0	n.q.	n.q.
Benzo(k)fluoranthene	1.5	2.7	n.q.	n.q.
Benzo(a)pyrene	5.2	3.8	n.q.	n.q.
Indeno[1,2,3-cd]pyrene	1.5	1.5	n.q.	n.q.
Dibenz[a,h]anthracene	1.5	1.5	n.q.	n.q.
Benzo[g,h,i]perylene	3.4	4.8	n.q.	n.q.
Benzene, pentachloro-	1.0	1.2	n.q.	n.q.
Benzene, hexachloro-	1.3	1.4	n.q.	n.q.
Lindane	97.9	147.2	n.q.	n.q.
Dieldrin	0.13	0.14	n.q.	n.q.

n.q. – not quantifiable

Table SI-7. TWA water concentrations calculated from spot samples and passive sampling data at the sampling site in the Meuse during the autumn campaign (Trial II).

Compound	Spot samples 14 days	Spot samples 28 days	Chemcatcher 14 days	Chemcatcher 28 days
Acenaphthene	0.4	1.5	12.5	11.2
Fluorene	0.7	1.0	7.4	11.9
Phenanthrene	3.9	4.7	6.6	13.2
Anthracene	0.2	0.8	n.q.	n.q.
Fluoranthene	10.4	13.5	6.4	13.7
Pyrene	24.0	31.3	12.8	17.1
Benz[a]anthracene	3.2	3.2	60.3	48.6
Chrysene	2.2	2.1	19.4	15.6
Benzo(b)fluoranthene	2.7	2.4	n.q.	n.q.
Benzo(k)fluoranthene	1.3	1.3	n.q.	n.q.
Benzo(a)pyrene	3.5	4.3	n.q.	n.q.
Indeno[1,2,3-cd]pyrene	4.0	4.6	n.q.	n.q.
Dibenz[a,h]anthracene	n.q.	n.q.	n.q.	n.q.
Benzo[g,h,i]perylene	10.4	13.4	n.q.	n.q.
Benzene, pentachloro-	n.q.	n.q.	n.q.	n.q.
Benzene, hexachloro-	0.03	0.02	n.q.	n.q.
Lindane	n.q.	n.q.	n.q.	n.q.
Dieldrin	n.q.	3.9	n.q.	n.q.

n.q. – not quantifiable

Table SI-8. TWA water concentrations calculated from spot samples and passive sampling data at the sampling site in the Alna during the spring campaign (Trial I).

Compound	Spot samples 14 days	Spot samples 28 days	Chemcatcher 14 days	Chemcatcher 28 days
Acenaphthene	1.0	1.1	8.0	11.0
Fluorene	1.7	1.7	9.5	9.6
Phenanthrene	5.4	5.2	11	16.4
Anthracene	1.6	1.7	0.9	2.4
Fluoranthene	6.0	6.2	n.q.	7
Pyrene	9.3	9.1	n.q.	8
Benz[a]anthracene	0.0	0.0	n.q.	n.q.
Chrysene	9.0	9.7	7	7
Benzo(b)fluoranthene	1.6	2.4	n.q.	n.q.
Benzo(k)fluoranthene	1.6	1.7	n.q.	n.q.
Benzo(a)pyrene	8.0	8.5	n.q.	n.q.
Indeno[1,2,3-cd]pyrene	3.1	3.3	n.q.	n.q.
Dibenz[a,h]anthracene	8.0	8.5	n.q.	n.q.
Benzo[g,h,i]perylene	8.0	8.5	n.q.	n.q.
Benzene, pentachloro-	1.6	1.7	n.q.	n.q.
Benzene, hexachloro-	1.6	1.7	n.q.	n.q.
Lindane	34.3	35.7	n.q.	n.q.
Dieldrin	1.6	1.7	n.q.	n.q.

n.q. – not quantifiable

Table SI-9. TWA water concentrations calculated from spot samples and passive sampling data at the sampling site in the Alna during the autumn campaign (Trial II).

Compound	Spot samples 14 days	Spot samples 28 days	Chemcatcher 14 days	Chemcatcher 28 days
Acenaphthene	0.7	0.5	10.4	3.1
Fluorene	0.8	0.6	9.7	4.6
Phenanthrene	2.0	1.9	13.2	7.2
Anthracene	0.7	0.8	5.0	3.9
Fluoranthene	2.0	2.0	19.9	18.8
Pyrene	0.8	0.5	18.2	18.1
Benz[a]anthracene	1.7	1.4	29.7	44.2
Chrysene	2.2	2.3	27.7	32.6
Benzo(b)fluoranthene	1.9	1.9	24.2	38.7
Benzo(k)fluoranthene	0.9	1.0	n.q.	n.q.
Benzo(a)pyrene	0.9	0.9	72.6	140.9
Indeno[1,2,3-cd]pyrene	0.8	0.8	n.q.	n.q.
Dibenz[a,h]anthracene	0.6	0.6	n.q.	n.q.
Benzo[g,h,i]perylene	1.7	1.7	n.q.	n.q.
Benzene, pentachloro-	0.1	0.2	n.q.	n.q.
Benzene, hexachloro-	0.1	0.3	n.q.	n.q.
Lindane	n.q.	n.q.	n.q.	n.q.
Dieldrin	1.0	0.62	n.q.	n.q.

n.q. – not quantifiable

Table SI-10. TWA water concentrations calculated from spot samples and passive sampling data at the sampling site in the Elbe during the spring campaign (Trial I).

Compound	Spot samples 14 days	Spot samples 28 days	Chemcatcher 14 days	Chemcatcher 28 days
Acenaphthene	n.q.	n.q.	n.q.	n.q.
Fluorene	1.10	1.5	1.3	1.6
Phenanthrene	6.3	7.1	n.q.	1.4
Anthracene	3.4	2.0	2.8	3.1
Fluoranthene		0.2	2.3	2.6
Pyrene	1.0	1.2	n.q.	n.q.
Benz[a]anthracene	n.q.	n.q.	8.1	6.8
Chrysene	n.q.	n.q.	n.q.	n.q.
Benzo(b)fluoranthene	n.q.	n.q.	n.q.	n.q.
Benzo(k)fluoranthene	n.q.	n.q.	n.q.	n.q.
Benzo(a)pyrene	n.q.	n.q.	n.q.	n.q.
Indeno[1,2,3- cd]pyrene	n.q.	n.q.	n.q.	n.q.
Dibenz[a,h]anthracene	n.q.	n.q.	n.q.	n.q.
Benzo[g,h,i]perylene	n.q.	n.q.	n.q.	n.q.
Benzene, pentachloro-	n.q.	n.q.	n.q.	n.q.
Benzene, hexachloro-	0.2	0.2	n.q.	n.q.
Lindane	n.q.	1.1	n.q.	n.q.
Dieldrin	n.q.	n.q.	n.q.	n.q.

n.q. – not quantifiable

Table SI-11. TWA water concentrations calculated from spot samples and passive sampling data at the sampling site in the Elbe during the autumn campaign (Trial II).

Compound	Spot samples 14 days	Spot samples 28 days	Chemcatcher 14 days	Chemcatcher 28 days
Acenaphthene	0.4	0.4	1.9	
Fluorene	0.4	0.5	2.1	1.8
Phenanthrene	5.9	5.8	7.5	6.6
Anthracene	0.2	0.2	4.7	0.3
Fluoranthene	2.3	2.1	3.4	3.1
Pyrene	2.5	2.3	2.8	2.5
Benz[a]anthracene	0.2	0.2	17.4	n.q.
Chrysene	0.4	0.4	n.q.	n.q.
Benzo(b)fluoranthene	0.1	0.1	n.q.	0.6
Benzo(k)fluoranthene	0.02	0.01	n.q.	n.q.
Benzo(a)pyrene	0.04	0.03	n.q.	n.q.
Indeno[1,2,3- cd]pyrene	0.1	0.1	n.q.	n.q.
Dibenz[a,h]anthracene	0.01	0.0	n.q.	n.q.
Benzo[g,h,i]perylene	0.1	0.1	n.q.	n.q.
Benzene, pentachloro-	n.q.	n.q.	0.1	0.1
Benzene, hexachloro-	0.1	0.1	0.3	n.q.
Lindane	1.2	1.2	3.4	3.4
Dieldrin	n.q.	n.q.	1.9	n.q.

n.q. – not quantifiable