

Contents

Contributors to Volume 48	vii
Volumes in the Series.	xi
Preface.	xxv
Series Editor's Preface	xxix
Foreword	xxxii

Part I: Air

Chapter 1. Theory of solid phase microextraction and its application in passive sampling

Yong Chen and Janusz Pawliszyn

1.1 Introduction	3
1.2 Calibration in solid phase microextraction.	6
1.2.1 Equilibrium extraction.	7
1.2.2 Exhaustive extraction.	8
1.2.3 Pre-equilibrium extraction	9
1.2.4 Calibration based on first-order reaction rate constant	10
1.2.5 Calibration based on diffusion	12
References	31

Chapter 2. The use of different designs of passive samplers for air monitoring of persistent organic pollutants

Rosalinda Gioia, Kevin C. Jones and Tom Harner

2.1 Introduction	33
2.2 The context: why develop passive air sampling techniques for POPS?	35
2.3 What approaches can be used?	38
2.4 The choice of sampler designs: features, advantages and potential problems	40
2.4.1 Low-capacity sampling: polymer-coated glass	42
2.4.2 Medium-capacity sampling devices: polyurethane foam disks	43
2.4.3 High-capacity sampling devices: semipermeable membrane devices and XAD-2 resin.	44

Contents

2.5	Case studies and applications of PAS for POPS.	46
2.5.1	POGs: case studies and applications.	46
2.5.2	SPMDs: case studies and applications.	47
2.5.3	PUF disks: case studies and applications.	49
2.5.4	XAD-2 resin: case studies and applications.	51
2.6	Future improvements and needs for PAS for POPS.	52
	References.	53

Chapter 3. Passive sampling in combination with thermal desorption and gas chromatography as a tool for assessment of chemical exposure

Anna-Lena Sunesson

3.1	The applicability of passive sampling for chemical exposure assessment.	57
3.2	Passive sampling, basic theory.	58
3.3	Sampling rates.	60
3.4	Standards for evaluation of passive samplers.	60
3.5	Sampler designs for passive sampling–thermal desorption analysis.	61
3.6	Thermal desorption.	64
3.7	Adsorbents.	67
3.8	Analytical equipment for thermal desorption.	69
3.9	Applications using passive sampling–thermal desorption–gas chromatography for exposure assessment; examples and trends.	70
3.10	Possible limitations/sources of error when using passive sampling–thermal desorption–gas chromatography.	72
3.11	Self-assessment of exposure.	74
3.12	Practical considerations.	76
3.12.1	Selecting a suitable adsorbent for the analytes of interest.	76
3.12.2	Minimising artefacts.	77
3.12.3	Blank samples.	78
3.12.4	Personal (individual) exposure assessment.	78
3.13	Concluding remarks and future perspectives.	79
	References.	79

Chapter 4. Use of permeation passive samplers in air monitoring

Bożena Zabiegaia and Jacek Namieśnik

4.1	Introduction.	85
4.2	Theory.	86
4.2.1	Membrane.	88

Contents

4.3	Design of the permeation passive sampler	91
4.4	Calibration of gut permeation passive samplers.	92
4.5	Determination of the calibration constants of gut permeation passive samplers with silicone membranes based on physico-chemical properties of the analytes	92
4.5.1	Number of carbon atoms	95
4.5.2	Molecular mass	96
4.5.3	Boiling point temperature	96
4.5.4	Linear temperature-programmed retention index system	98
4.5.5	Application of GUT permeation passive sample in indoor air analysis	103
4.6	Conclusion	104
	References	105

Chapter 5. Membrane-enclosed sorptive coating as integrative sampler for monitoring organic compounds in air

Peter Popp, Heidrun Paschke, Branislav Vrana, Luise Wennrich and Albrecht Paschke

5.1	Introduction	107
5.2	Theory	108
5.3	Experimental	110
5.3.1	Preparation and design of the MESCO samplers	110
5.3.2	Chemicals	111
5.3.3	Generation of the standard gas mixtures and calibration of the samplers.	111
5.3.4	Thermodesorption/GC-MS analysis	114
5.3.5	Field application.	116
5.4	Results	116
5.4.1	Laboratory exposure experiments.	116
5.4.2	Comparison of the different MESCO types	118
5.4.3	On-site exposure experiments.	119
5.5	Conclusions.	122
	References	122

Chapter 6. Towards quantitative monitoring of semivolatile organic compounds using passive air samplers

Michael E. Bartkow, Carl E. Orazio, Todd Gouin, James N. Huckins and Jochen F. Müller

6.1	Introduction	125
6.2	Estimating air concentrations.	126

Contents

8.5.2	Comparison of POCIS and traditional sampling for wastewater monitoring.	186
8.5.3	Application of POCIS for pesticide monitoring in Denmark	187
8.5.4	Application of POCIS for pharmaceutical monitoring in the United Kingdom.	189
8.6	Future research consideration.	192
8.6.1	Development of the PRC approach in POCIS	192
8.6.2	Determination of sampling rate and kinetic data for chemicals of interest	194
8.7	Conclusions	195
	References	196

Chapter 9. Monitoring of priority pollutants in water using Chemcatcher passive sampling devices

Richard Greenwood. Graham A. Mills. Branislav Vrana. Ian Allan, Rocío Aguilar-Martinez and Gregory Morrison

9.1	Introduction	199
9.2	Concept of Chemcatcher	199
9.2.1	Receiving phases	200
9.2.2	Diffusion membranes	201
9.2.3	Sampler body	203
9.3	Theory	206
9.4	Calibration	207
9.5	Sampling of hydrophobic organic contaminants.	207
9.5.1	Calibration data	208
9.5.2	Performance reference compound concept	210
9.5.3	Non-polar Chemcatcher/water distribution coefficients	211
9.5.4	Empirical uptake rate model	211
9.5.5	Estimation of <i>in situ</i> TWA concentrations	212
9.6	Sampling of hydrophilic organic contaminants	213
9.6.1	Integrative sampler	213
9.6.2	Short pollution event detector	215
9.7	Sampling of metals	216
9.8	Sampling of organometallic compounds.	217
9.9	Field applications	217
9.9.1	Pan-European field trials to compare the performances of the Chemcatcher and spot sampling in monitoring the quality of river water.	217
9.9.2	Monitoring pesticide runoff in Brittany, France	219

Contents

9.9.3	Field trial in the River Meuse in The Netherlands . . .	220
9.9.4	Field trial in the estuary of the River Ribble in the United Kingdom.	222
9.10	Comparison of the performance of the Chemcatcher with that of other sampling devices.	223
9.11	Future trends	226
	Acknowledgments	226
	References	227
 <i>Chapter 10. Membrane-enclosed sorptive coating for the monitoring of organic compounds in water</i>		
Albrecht Paschke, Branislav Vrana, Peter Popp, Luise Wennrich, Heidrun Paschke and Gerrit Schuurmann		
10.1	Introduction	231
10.2	Passive uptake model for MESCO sampler	232
10.3	Design of the different MESCO formats	233
10.3.1	PDMS-coated fibre enclosed in an LDPE membrane	233
10.3.2	PDMS-coated stir bar enclosed in a dialysis membrane bag (MESCO I)	233
10.3.3	Silicone material enclosed in an LDPE membrane (MESCO II)	234
10.4	Laboratory-derived sampling rates of the various MESCO formats	235
10.5	Field application of MESCO samplers	237
10.5.1	A case study with MESCO I for monitoring of persistent organic pollutants in surface water.	237
10.5.2	Field trials with MESCO 11—first results	246
	Acknowledgments	248
	References	248
 <i>Chapter 11. In situ monitoring and dynamic speciation measurements in solution using DGT</i>		
Kent W. Warnken, Hao Zhang and William Davison		
11.1	Introduction	251
11.2	Methodology	253
11.2.1	Gel preparation	253
11.2.2	Diffusive gel variants	254
11.2.3	Alternative binding agents	254
11.3	DGT theory.	256
11.3.1	DGT principles.	256
11.3.2	Potential sources of error when using DGT	257

Contents

11.4	Novel applications	263
11.4.1	Analytes	263
11.4.2	Kinetics	265
11.4.3	Speciation	266
11.4.4	Bioavailability	271
11.4.5	The use of DGT as a routine monitoring tool	273
11.4.6	Metal remobilization from settling particles	274
11.5	Conclusion	274
	References	275

Chapter 12. Use of ceramic dosimeters in water monitoring

Hansjörg Weiß, Kristin Schirmer, Stephanie Bopp and Peter Grathwohl

12.1	Introduction	279
12.2	Ceramic dosimeter design	280
12.2.1	Ceramic membrane	280
12.2.2	Sorbent material	282
12.2.3	Determination of time-weighted average chemical concentrations	283
12.2.4	Effect of temperature	285
12.3	Practical considerations	285
12.3.1	Preparation of the ceramic dosimeter for field application	285
12.3.2	Sampling rates	286
12.3.3	Detection limits	287
12.3.4	Long-term stability	289
12.4	Example of field results and future work	290
	Acknowledgment	292
	References	292

Chapter 13. Passive diffusion samplers to monitor volatile organic compounds in ground-water

Don A. Vroblesky

13.1	Introduction	295
13.2	Applications	299
13.2.1	VOCs in ground-water at the ground-water/surface-water interface	299
13.2.2	VOCs in ground-water in monitoring wells	302
13.3	Conclusions	306
	Acknowledgment	307
	References	307

Contents

Chapter 14. Field study considerations in the use of passive sampling devices in water monitoring

Per-Anders Bergqvist and Audrone Zaliauskiene

14.1	Introduction	311
14.1.1	SPMD rationale and applicability	312
14.2	Field study considerations	315
14.2.1	Pre-exposure considerations	315
14.2.2	SPMD storage considerations	322
14.2.3	Precautions/procedures during deployment and retrieval of SPMDs	323
14.3	Quality control	325
	References	327

Chapter 15. Techniques for quantitatively evaluating aquatic passive sampling devices

B. Scott Stephens and Jochen F. Müller

15.1	Introduction	329
15.2	Key parameters	330
15.2.1	Equilibrium partitioning	330
15.2.2	Time-integrated sampling	330
15.3	Laboratory methods	331
15.3.1	The concentration problem	331
15.3.2	Batch techniques	331
15.3.3	Flow through techniques	335
15.4	<i>In situ</i> methods	338
15.4.1	High-volume solid-phase extraction	339
15.4.2	Grab sampling validation methods	341
	References	346

Part III: Soils and Sediments

Chapter 16. Theory and applications of DGT measurements in soils and sediments

William Davison, Hao Zhang and Kent W. Warnken

16.1	Introduction	353
16.2	Principles in soils and sediments	354
16.3	Modelling interactions of DGT with soils and sediments	357
16.4	Soils	360
16.4.1	Practicalities for deployments in soils	360

Contents

16.4.2	Soil dynamics	361
16.4.3	Biological mimicry	363
16.5	Sediments	367
16.5.1	Practicalities for deployments in sediments.	368
16.5.2	Analyte distributions from gel slicing	369
16.5.3	Direct measurements of analytes in the binding layer	371
16.5.4	Sources of localised maxima	373
16.5.5	Advances in understanding of soils and sediments using DGT	374
References	374

Chapter 17. Passive sampling devices for measuring organic compounds in soils and sediments

Gangfeng Ouyang and Janusz Pawliszyn		
17.1	Introduction	379
17.2	PETREX passive soil gas and sediment vapour sampling system	380
17.3	GORE TM modules for passive soil gas collection	381
17.4	Emflux [®] passive soil gas sampling system.	382
17.5	Semipermeable membrane devices for passive sampling in sediment pore-water	383
17.6	Solid-phase microextraction devices for passive sampling in soil and sediment	384
17.7	Conclusion	388
References	389

Part IV: Ecotoxicology and Biomonitoring

Chapter 18. Use of passive sampling devices in toxicity assessment of groundwater

Kristin Schirmer, Stephanie Bopp and Jacqueline Gehrhardt		
18.1	Introduction	393
18.2	Concepts and examples for linking passive sampling of groundwater with toxicological analysis.	394
18.2.1	The toximeter	396
18.2.2	Toxicological analysis of solvent extracts obtained from passive sampling devices.	401
18.3	Potential future approaches	403
Acknowledgments.	404
References	404