

# Training Course on Passive Sampling

Speaker: Dr Kees Booij (PaSOC)



Passive sampling has been shown to be a suitable alternative to traditional sampling techniques to overcome sensitivity and representativeness issues encountered in measuring low and fluctuating aqueous concentrations. In response to increasing interest in this method, a training course is organized by the University of Lausanne in March 14 – 16, 2018. This course will be given by Dr Kees Booij who is involved in passive sampling research since 1995 (see CV below). Participants have the opportunity to register for one, two or three days according to their interest in the proposed modules. Some time slots will be dedicated to experience sharing among participants (exposition, posters, informal discussion...).

## Target audience

- **Practitioners and project managers** interested in designing monitoring campaigns based on passive sampling.
- **PhD students and researchers** who want to deepen their understanding of water-sampler exchanges to address research challenges.

## Objectives

- **Day 1:** ability to conceptually link passive and active sampling, choose appropriate samplers and have qualitative understanding of uncertainties
- **Day 2:** understanding how exposure conditions impact the uptake and how uncertainties associated to the use of calibration results in field studies can be reduced
- **Day 3:** experiments required to improve the quality of passive sampler calibration and the mechanistic understanding of exchanges

## Practical information

- **Organizer:** School of Criminal Justice of the University of Lausanne (Faculty of Law, Criminal Justice and Public Administration)
  - **Location:** Amphipôle building, room 342 (see access information on last page)
  - **Duration:** 1 to 3 days
  - **Dates:** Wed 14 - Fri 16 March
  - **Registration:** at [nicolas.estoppey@unil.ch](mailto:nicolas.estoppey@unil.ch), as soon as possible (number of participants is limited to 32), but before February 10<sup>th</sup>
  - **Price** (incl. lunches and coffee breaks):
    - 1 day: 200 euros
    - 2 days: 320 euros
    - 3 days: 400 euros
- Payment before February 10<sup>th</sup> (see payment information on last page)
- **Contribution:** If you wish to present a poster, or bring passive sampling materials, please contact us at [nicolas.estoppey@unil.ch](mailto:nicolas.estoppey@unil.ch)

# Course program

## Day 1

10:15 - 10:30 *Introduction*

10:30 - 12:00 **Module 1: Overview of passive samplers**

Samplers for organic compounds (volatile, nonpolar, polar) and metals.  
Principles of operation, similarities and differences, case studies.

12:00 - 13:30 *Lunch*

13:30 - 15:00 **Module 2: Performance characteristics**

Sampling rates, sorption capacities, time-integrative windows, detection limits, sampler selection criteria, uncertainties.

15:00 - 15:30 *Coffee break*

15:30 - 17:30 **Module 3: Practical aspects**

Quality assurance & quality control, considerations for field studies.

**Poster presentations + examples of samplers and exposure devices**

If you are interested in presenting a poster, or bringing passive sampling materials, please contact us at [nicolas.estoppey@unil.ch](mailto:nicolas.estoppey@unil.ch)

## Day 2

09:00 - 10:30 *Posters + coffee + informal discussions*

10:30 - 12:00 **Module 4: Uptake rate control**

Effect of transport through the water boundary layer, membrane/polymer, sorbent on the uptake rates.

12:00 - 13:30 *Lunch*

13:30 - 15:00 **Module 5: Passive sampler calibration**

Laboratory calibration methods for partition coefficients and sampling rates.  
In situ calibration of samplers for nonpolar compounds.

15:00 - 15:30 *Coffee break*

15:30 - 17:00 **Module 6: Accounting for the effect of hydrodynamics on polar organic compound uptake**

Structure of the water boundary layer, hydrodynamical models, experimental methods to measure water boundary layer resistance.

## Day 3

09:00 - 10:30 *Posters + coffee + informal discussions*

10:30 - 12:00 **Module 7: Going more deeply into models**

Transport resistance model, partial rate control by water boundary layer and membrane, non-steady state sampling rates, generalised model for boundary layer controlled mass transfer in closed and open systems. Transport in porous membranes. Model assumptions, limitations, and prospects.

12:00 - 13:30 *Lunch*

13:30 - 15:00 **Module 8: Programming and developing**

Modelling of partial and complete polymer controlled uptake. Determination of diffusion coefficients in polymers and polymer-polymer partition coefficients.

15:00 - 15:30 *Coffee break*

15:30 - 17:00 **Module 9: Research and communication challenges**

Quantifying and communicating uncertainty, standardisation and harmonisation of methods, dealing with the effects of exposure conditions. Atrazine case study. Relationships between physicochemical properties and sampling rates. Other knowledge gaps. Group discussion.

## Day 1

Day 1 is for a general overview of which samplers are available, and what they can and cannot do. The conceptual link between passive and active sampling is presented. The concepts of sampling rate, sorption capacity, time-integrative window are introduced. Methods to evaluate if a particular sampler can fulfil the needs of a particular monitoring study are discussed, including the estimation of uncertainties and the design of field monitoring studies. Model equations are made plausible, without going into details of model derivations.

### **Module 1: Overview of passive samplers**

Passive samplers accumulate analytes of interest by ambient diffusion and advection. Although their principle of operation is similar, many different configurations exist. These samplers can be broadly categorised depending on the group of analytes that are sampled: 1. volatile organic compounds, 2. polar and ionic organic compounds, 3. nonpolar organic compounds, and 4. metals and nutrients. An overview will be given of these four main sampler classes. Several frequently used devices will be discussed in more detail. Their performance will be illustrated using a number of case studies. Data evaluation as well as strengths and weaknesses will be summarised.

### **Module 2: Performance characteristics**

A first screening of the usefulness of a particular passive sampler for a monitoring study can be based on two performance characteristics that are easily obtained: the water sampling rate and the sorption capacity. The water sampling rate is the equivalent water volume that is extracted per unit time at the initial stages of sampler exposure. The sorption capacity is the equivalent water volume that is extracted when the sampler reaches equilibrium with the surroundings. Both concepts yield valuable information on the achievable detection limits and on the sampler's ability to yield time weighted average concentrations. In addition, these concepts provide a conceptual link between batch sampling and passive sampling. This first screening of passive sampler performance can be done without complex modelling, as illustrated with some examples.

Other passive sampler features are important as well, such as cost, ease of use, and commercial availability. In addition, the uncertainty in the obtained concentration estimates is highly relevant information. Uncertainties arise from the chemical analysis of the sampler, the quality of the calibration parameters, the effect of exposure conditions on sampling rate and sorption capacity, and the quality of the models that are used for converting absorbed amounts to aqueous concentrations. The importance of these factors for the overall uncertainties will be discussed. Considerations for comparing uncertainties between batch sampling and passive sampling will be presented.

### **Module 3: Practical aspects**

A number of guidelines exist for the design of passive sampling based monitoring. These guidelines aim to maximise the success of field studies and the quality of the obtained information. Next to considerations that apply to monitoring studies in general, several aspects will be highlighted that are specific for passive sampling based monitoring, such as the use of control samplers, documentation of exposure conditions, sampler storage and transport, and data reporting.

As part of this module, participants will be taken along a number of samplers and exposure devices (hands on). If you are interested in bringing your own passive sampling materials, please contact us at [nicolas.estoppey@unil.ch](mailto:nicolas.estoppey@unil.ch).

## Day 2

Day 2 is for users who want to go one step deeper. The focus will be on passive sampler calibration, application of calibration results in field studies, and the effect of exposure conditions on sampling rates. The available models will be interpreted in terms of basic physical principles, without going into great mathematical detail.

### **Module 4: Uptake rate control**

The uptake of chemicals by passive samplers includes transport through the water boundary layer, the membrane (if present) and the receiving phase (sorbent or polymer). Each of these steps can be rate limiting. Understanding of the rate limiting transport steps is important for developing mechanistic relationships between accumulated amounts and aqueous concentrations. These relationships are needed to understand the effect of exposure conditions (flow, temperature) and sampler design features (e.g., membrane thickness, choice of sorbent or polymer) on the uptake rates. The transport resistance model is a straightforward approach to the interpretation of calibration data. This model treats the overall transport resistance as a sum of the resistances for transport through the boundary layer, the membrane and the sorbent. The model works best when the sampling can be characterised by a sampling rate that is independent of time. Strengths and limitations of the transport resistance model will be discussed using literature data and the results of more complex diffusion models.

### **Module 5: Passive sampler calibration**

The availability of reliable calibration data is crucial for the successful application of passive sampling in environmental monitoring. This calibration data is also important for enhancing our mechanistic understanding of the accumulation process. Knowledge of the sampler-water partition coefficients is needed for chemicals that reach partial or complete sampler-water equilibrium. Knowledge of sampling rates is needed for chemicals that typically remain in the linear uptake stage of the sampling process. Laboratory calibration setups can be distinguished in single dose, multiple dose, and flow through designs. Dominant features, and strengths and weaknesses of these designs will be discussed. Special attention will be given to the behaviour of passive samplers in small water volumes as compared with sampling in the environment, where water volumes are essentially infinite. Challenges with translating laboratory derived calibration parameters to field exposures will be discussed. The options for in-situ calibration of sampling rates with performance reference compounds will be presented.

### **Module 6: Accounting for the effect of hydrodynamics on polar organic compound uptake**

Water flow velocities in the environment range from essentially zero to several metres per second. Although the sensitivity of sampling rates to changes in flow velocity can be very different, all sampling rates are controlled by the water boundary layer when the flow gets smaller and smaller. Exact hydrodynamical models for mass transfer only exist for simple flow configurations. However, the flow near the sampler surface is usually very complex and alternative approaches to account for flow effects on sampling rates are needed. These approaches include semi-empirical models that are used in the engineering literature, computational fluid dynamics, and experimental methods to directly measure the boundary layer resistance.

*For day 2, a computer equipped with Excel® software could be helpful for practical exercises*

## Day 3

Day 3 is targeted at researchers who aim to further develop the understanding and application of passive sampling methods. A number of more complex models for sampler-water exchange will be presented. Research and communication challenges will be highlighted. Knowledge gaps and directions for future research will be discussed.

### **Module 7: Going more deeply into models**

Several frequently used models for sampler-water exchange are special cases of more general models. For example, the models for boundary layer controlled uptake and release of chemicals between polymers and water are governed by the same differential equations, and differ only in the initial conditions that apply. Similarly, the models for uptake and release in infinite water volumes are limiting cases of more general models that apply for finite water volumes. Further, models for transport within a polymer and transport through the channels in a porous membrane are special cases of a more general model that allows for transport both via the pore space and via the polymer matrix. The background, model assumptions, and implications of these models for understanding sampling rates will be discussed.

### **Module 8: Programming and developing**

Models for partial or complete rate control by the polymer/membrane/sorbent are typically much more complex than models for boundary layer controlled exchange. The same holds for the determination of diffusion coefficients within polymers and for transport between two or more polymers. A number of mathematical methods for dealing with these cases will be presented. Their implementation in spreadsheet programs will be illustrated.

### **Module 9: Research challenges**

Although great progress has been made in our mechanistic understanding of passive sampling, a number of processes require further study and maturation. A further challenge is that the application of passive sampling in regulatory monitoring is somewhat disappointing in view of the progress that is made during nearly three decades of extensive scientific research. Possible reasons for this less than optimal use of passive sampling may be that the concerns of regulators have not been fully appreciated by academia. In addition, the achievements and shortcomings of passive sampling may not have been communicated clearly enough. A list of possible research and communication challenges will be presented. This list includes (but is not limited to) communicating uncertainty, standardisation of calibration methods and sampler designs, harmonisation and cross-calibration of passive sampling methods, dealing with the effects of exposure conditions (flow, temperature, biofouling), understanding and prediction of sampling rates and partition coefficients from physicochemical properties, and rate control by the sorbent. Course participants are invited to share and discuss their ideas on these issues in an active group discussion.

*For day 3, a computer equipped with Excel® software could be helpful for practical exercises*

# Kees Booij



Kees Booij obtained MSc's in physical chemistry (1983, VU University, Amsterdam) and chemical engineering (1985, University of Amsterdam). He started his PhD research at the Netherlands Institute of Sea Research (NIOZ) on exchange of oxygen and polychlorinated biphenyls between sediment and water, followed by a PhD defence at the University of Groningen (1989).

From 1989 - 2016 he worked as a scientist at the Netherlands Institute for Sea Research, with a focus on the environmental chemistry of organic contaminants. In 2016 he started the company Passive Sampling of Organic Compounds - PaSOC, working as a free-lance passive sampling scientist. He authored/co-authored 55 publications in the peer-reviewed literature, one book, and two book chapters.

He is a member of the Marine Chemistry Working Group of the International Council for the Exploration of the Sea, and he is a member of the editorial board of Environmental Toxicology and Chemistry. His main scientific focus over the past 20 years has been passive sampling of organic compounds. Further details can be found at:

- <http://www.pasoc.eu>
- <http://orcid.org/0000-0002-3962-3155>
- <http://www.researcherid.com/rid/K-5413-2015>

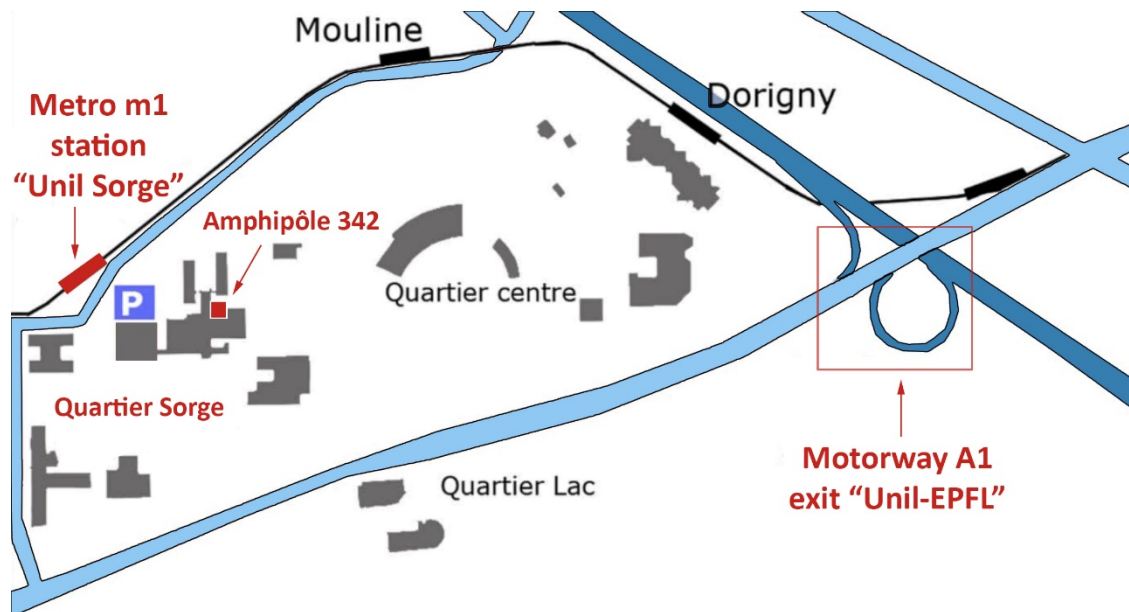
## PaSOC

PaSOC seeks to improve science-based assessments of the exposure of humans and the environment to organic compounds, specifically by advancing the knowledge of passive sampling, and promoting its application in such assessments. PaSOC is a sole proprietorship.



PaSOC operates at the interface between science and application by closely monitoring the scientific passive sampling literature, and by listening carefully to the needs of those involved in the practical application of passive sampling methods in a regulatory context. PaSOC aims to feed newly developed knowledge into the world of applied science, and to feed unresolved challenges into the world of the more fundamental science. To this end, PaSOC maintains a global network of partners from academia, industry, and governmental organisations.

# Access information



## By train:

From Lausanne railway station:

- Metro m2 (direction: "Croisettes") to "Lausanne-Flon"
- Then, metro m1 (direction: "Renens") to "UNIL-Sorge"

From Renens railway station:

- Metro m1 (direction: "Lausanne-Flon") to "UNIL-Sorge"

## By car:

- Motorway, direction "Lausanne-Sud"
- Exit "UNIL-EPFL"
- To "Quartier Sorge", parking Sorge

## By plane:

- To Geneva airport
- Then, by train to Lausanne or Renens

# Payment information

Please, make the payment to the following bank account before February 10th (mention: "Passive Sampling / Fonds 2602 5867"):

Ecole des Sciences Criminelles  
BANQUE CANTONALE VAUDOISE  
1002 Lausanne  
(CCP 10-725-4)

Account number: 352.87.60  
Clearing number: 767  
SWIFT: BCVLCH2L  
IBAN : CH38 0076 7000 U035 2876 0

# Accommodation suggestions

## On the campus:

- SwissTech Hotel
- Starling Hotel

## In Lausanne (limited budget):

- Lausanne Youth Hostel Jeunotel
- Hotel Ibis Lausanne Center