

# **$C_w$ calculation template for passive samplers of hydrophobic compounds**

## **Background information and manual**

7 July 2023

Kees Booij



Passive Sampling of Organic Compounds / PaSOC

Grote Pierwei 25, 8821LV Kimsward, The Netherlands

[www.pasoc.eu](http://www.pasoc.eu)

[info@pasoc.eu](mailto:info@pasoc.eu)

## Table of Contents

Abstract	2
1. Scientific background	3
Sampling rates	3
Sampler-water partition coefficients	4
Temperature and salinity effects on $K_{sw}$	4
2. Use of the $C_w$ calculation template	5
Properties worksheet	5
$C_w$ worksheet	5
Block 1 : Method information	6
Block 2: Exposure data	6
Block 3: PRC data	6
Block 4: Accumulated amounts	7
Block 5: Results	7
Block 6: $C_w$ summary	9
Note on replication	9
3. Template validation	9
4. Further support	10
5. Terms of use	10
6. Changes compared with previous version	10
7. References	11

## Abstract

This document provides background information and instructions for use of an Excel template for calculating aqueous concentrations from amounts in passive samplers of hydrophobic compounds. The sampling rate model is based on water boundary layer controlled uptake rates. Sampler-water partition coefficients are obtained from experimental values. Justification for the use of these models is discussed.

## 1. Scientific background

Passive samplers for hydrophobic compounds have been used for many years to monitor concentrations of freely dissolved compounds in water. These concentrations ( $C_w$ ) can be calculated from the accumulated amounts ( $N$ ) by (Huckins et al., 2006; Smedes and Booij, 2012)

$$C_w = \frac{N}{m_s K_{sw} \left[ 1 - \exp\left(-\frac{R_s t}{m_s K_{sw}}\right) \right]} \quad 1$$

where  $t$  is time,  $R_s$  is the water sampling rate,  $K_{sw}$  is the sampler-water partition coefficient (volume per mass units) and  $m_s$  is the sampler mass. When  $K_{sw}$  is given in volume per volume units, then the sampler volume ( $V_s$ ) should be used instead of  $m_s$ . The accumulated amounts are determined by chemical analysis, and  $m_s$  is determined by weighing. Application of eq. 1 requires knowledge of and  $R_s$  and  $K_{sw}$ , as discussed below.

### Sampling rates

Sampling rates depend on flow and temperature. The performance reference compound (PRC) method is used for the in-situ calibration of the uptake kinetics (Booij and Smedes, 2010; Huckins et al., 2002). PRCs are compounds of moderate hydrophobicity ( $\log K_{ow}$  typically in the range 4 to 6) that do not occur in the environment, and are spiked into the samplers prior to deployment. The amounts of these compounds in the sampler ( $N$ ) follow an exponential decrease with time

$$f = \frac{N}{N_0} = \exp\left(-\frac{R_s t}{m_s K_{sw}}\right) \quad 2$$

where  $N_0$  is the amount present in the samplers at  $t = 0$  (determined from analysis of unexposed samplers),  $f$  is the PRC fraction that is retained during the exposure. For sampling of hydrophobic chemicals, the sampler-water exchange kinetics are generally controlled by transport through the water boundary layer (WBL). In this case,  $R_s$  is proportional to the diffusion coefficient in water ( $D_w$ ) to the power 2/3 (Booij et al., 2003; Booij and Smedes, 2010). Schwarzenbach et al. (2003) showed that molecular weight can be used as a predictor of  $D_w$  at 25 °C

$$D_w = \frac{2.7 \times 10^{-8}}{MW^{0.71}} \quad 3$$

where  $D_w$  is given in  $m^2/s$ . The  $R_s$  for WBL controlled kinetics is therefore inversely proportional to the molecular weight to the power  $0.71 \times 2/3 = 0.47$

$$R_s = \frac{\beta_M}{MW^{0.47}} \quad 4$$

where  $\beta_M$  reflects the exposure-specific effect on  $R_s$ , and  $MW$  takes the compound-specific effect on  $R_s$  into account. Putting everything together, PRC dissipation can be modelled by

$$f = \frac{N}{N_0} = \exp\left(-\frac{\beta_M t}{m_s K_{sw} MW^{0.47}}\right) \quad 5$$

$\beta_M$  is obtained by nonlinear least squares estimation of  $f$  as a function of  $K_{sw} MW^{0.47}$ . Aqueous concentrations of the target chemicals can be calculated from

$$C_w = \frac{N}{m_s K_{sw} \left[ 1 - \exp\left(-\frac{\beta_M t}{m_s K_{sw} MW^{0.47}}\right) \right]} \quad 6$$

WBL controlled exchange kinetics can be assumed when

$$\frac{R_s L}{AD_p K_{sw} \rho_s} \ll 3 \quad 7$$

where  $A$  is the surface area of the sampler ( $2 \times \text{length} \times \text{width}$ ),  $L$  is the half-thickness,  $\rho_s$  is the sampler density, and  $D_s$  is the diffusion coefficient in the polymer. With samplers of hydrophobic compounds (e.g., silicone, LDPE, SPME), the left hand side of eq. 7 is typically (much) smaller than 0.01 for nonpolar compounds (PCBs, PBDEs, PAHs, pyrethroids) and slightly polar compounds (DDTs, HCHs, drins) (Booij, 2021). These samplers are not so useful for sampling of compounds with low  $\log K_{ow}$  values, because these analytes also have small  $K_{sw}$  values (<100) and quickly reach sampler-water equilibrium, which challenges the samplers' ability to yield time-integrated aqueous concentrations.

### Sampler-water partition coefficients

Experimental  $K_{sw}$  values are preferred over values that are based on correlations with  $\log K_{ow}$  or linear free energy relationships (LFERs). Experimental  $K_{sw}$  values for a variety of nonpolar and polar compounds are available for silicone (Grant et al., 2016; Kwon et al., 2007; Smedes, 2019; Smedes et al., 2009; Smedes and Beeltje, 2010), LDPE (Lei et al., 2020; Lohmann, 2012; Pintado-Herrera et al., 2016; Reitsma et al., 2013; Smedes et al., 2009), and SPMDs (Huckins et al., 2006; Smedes, 2019). Many more  $K_{sw}$  data are available from other references. Some  $\log K_{sw}$  values are included in the template for the convenience of the user. Accuracy of  $K_{sw}$  is only critical for chemicals that attain partial or complete equilibrium during the exposure, i.e. for PRCs and for chemicals with  $\log K_{sw}$  values < 6. The more hydrophobic compounds generally reach an insignificant degree of equilibrium during typical exposure periods of 3 to 6 weeks, and uncertainties in their  $K_{sw}$  values have a negligible effect on the accuracy of the measured aqueous concentrations. Special care is needed with the selection of  $\log K_{sw}$  values for silicone samplers, because considerable differences ( $\sim 0.3$  log units) have been observed among silicone types (Gilbert et al., 2016; Smedes et al., 2009). With SPMDs, the  $\log K_{sw}$  values reported by Huckins et al. (2006) for compounds with  $\log K_{ow} > 5.5$  are probably artificially low (Booij et al., 2014; Smedes, 2019).

When experimental values are not available, PaSOC is happy to estimate  $K_{sw}$  from  $K_{ow}$  and/or LFERs, if needed.

### Temperature and salinity effects on $K_{sw}$

Lower temperatures and higher salinities result in higher  $K_{sw}$ . A temperature decrease by 10 °C causes  $K_{sw}$  to increase by a factor of 1.15 to 2.5, and this increase is generally larger for the more hydrophobic compounds (Jonker et al., 2015; Lohmann, 2012).  $K_{sw}$  values in seawater can be a factor of 1.5 larger in seawater as compared with freshwater (Jonker et al., 2015).

Present template does not account for temperature and salinity effects on  $K_{sw}$  for several reasons. First, ignoring the effects of lower temperatures causes an overestimation of  $C_w$ . However, bioaccumulation factors of nonpolar compounds are also larger at lower temperature (Muijs and Jonker, 2009). This means that the overestimated  $C_w$  still gives a fair prediction of bioaccumulation potential when bioaccumulation factors at 20 °C are used (Ghosh et al., 2014, Supplemental data, page 4). Second, the parameters that are needed to make temperature and salinity corrections are not abundant, and not readily available for many compounds of interest. Third, overestimation of  $C_w$  at lower temperature and higher salinity is relatively independent of location and compound hydrophobicity (Jonker et al., 2015, Figures S6 and S7A). Bottom line of these considerations is that neglecting the effects of temperature and salinity does not greatly affect the accuracy of passive sampling based monitoring, although PaSOC is happy to adapt the template to account for temperature and salinity effects, if needed.

## 2. Use of the $C_w$ calculation template

Save a read-only copy of the template as a backup, before making changes.

### Properties worksheet

The “Properties” worksheet contains compound names, CAS numbers, values for molecular weight, and  $\log K_{sw}$  data from several literature sources. These values are supplied for the consideration of the user. Column E contains the  $\log K_{sw}$  values that are used in the calculations, which may be replaced with other values as required. Selection of optimal  $\log K_{sw}$  is the responsibility of the user.

compound group	compound	CAS	MW	selected $\log K_{sw}$	selected source
Rows between the highlighted rows can be inserted, deleted, or re-ordered as needed. Do not delete the highlighted rows.					
PCBs	PCB 1	2051-60-7	188.7	4.04	Smedes 2019
PCBs	PCB 2	2051-61-8	188.7	4.18	Smedes 2019
PCBs	PCB 3	2051-62-9	188.7	4.15	Smedes 2019
PCBs	PCB 4	13029-08-8	223.1	4.20	Smedes 2019
PCBs	PCB 10	33146-45-1	223.1	4.35	Smedes 2019
PCBs	PCB 14	34883-41-5	223.1	4.81	Smedes 2019
PCBs	PCB 18	37680-65-2	257.5	4.95	Smedes 2019
PCBs	PCB 21	55702-46-0	257.5	5.14	Smedes 2019

Compound names may be changed according to user preference.

Cells in columns B, D, and F are used to retrieve data for the  $C_w$  calculation in worksheet “Cw”. Columns to the right of column F are used to store data from various sources. Change the  $\log K_{sw}$  values as required (use copy from the right, or use a cell reference to values at the right).

Rows may be deleted, moved, copied, or inserted as required, but do not delete the highlighted rows.

Always Cut/Insert/Paste/Delete complete rows.

### $C_w$ worksheet

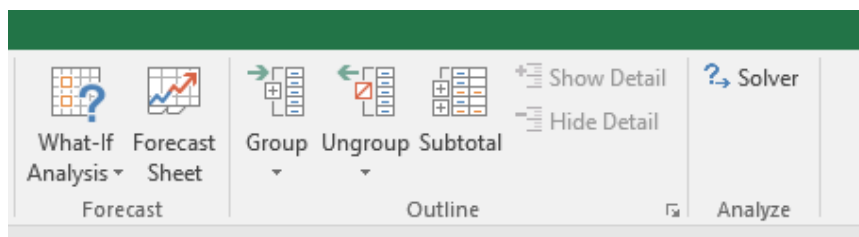
Rows 1-117 are hidden for convenience of the user. These rows are not locked or protected, and may be unhidden when required.

Columns A-W are used for input data (PRC fractions and amounts of target compounds). Model output is shown in columns AA-AW.

Cells with a green background should be filled out by the user. The other cells should not be changed.

A maximum of 20 exposures can be processed together.

Check that the solver add-in is activated (Data tab, far right, should display the word “Solver”)



**Block 1 : Method information**

This part contains a summary of the model and the source of the  $K_{sw}$  data.

<b>Block 1</b>				
<b><math>R_s</math> model</b>				
model eq.			$R_s = \beta_M / MW^{0.47}$	
model ref.			Rusina et al. ES&T 44: 362–367, 2010	
adjustable parameter	$L d^{-1} g^{0.47} mol^{-0.47}$	$\beta_M$		
<b><math>K_{sw}</math> data</b>				
			retrieve from worksheet "properties"	

**Block 2: Exposure data**

<b>Block 2</b>				
<b>Exposure data</b>				
Exposure ID			site1	site2
exposure time		d	27	27
sampler mass		kg	0.0034	0.0035
sampler surface area		dm <sup>2</sup>	0.99	0.99

Exposure ID: Any name

Exposure time in days.

Sampler mass in kg.

Sampler surface area: exchange surface area ( $2 \times \text{length} \times \text{width}$ ). This is used to calculate surface area normalised sampling rates.

**Block 3: PRC data**

Twenty rows with PRC data can be used in the calculations.

Keep the number of rows at 20; do not insert or delete rows from this block. Do not sort or move rows within this block.

Rows that are left blank are ignored.

<b>Block 3</b>				
<b>Retained PRC fractions</b>				
PRC name	$MW$	$\log K_{sw}$	$f_{obs}$	$f_{obs}$
fluorene-D10	176.20	3.44	0.000	0.000
anthracene-D10	188.20	3.88	0.000	0.000
pyrene-d10	212.25	4.34	0.032	0.032
chrysene-d12	240.36	4.80	0.311	0.356
PCB 10	223.10	4.35	0.034	0.039
PCB 30	257.54	5.01	0.520	0.504
PCB 104	326.43	5.88	0.864	0.941
PCB 145	360.88	6.44	1.007	0.954
PCB 204	429.77	7.43	1.019	1.043
PCB 170	not used	not used		
PCB 180	not used	not used		
PCB 182	not used	not used		
PCB 187	not used	not used		
PCB 189	not used	not used		
PCB 204	not used	not used		
PCB 206	not used	not used		
PCB 209	not used	not used		

Specify the name of the PRCs in the first column by selecting compound name from the drop-down list. Changes in compound names and list order should be made in the worksheet "Properties".

Compounds may be added to, or removed from to the drop-down list, by inserting/deleting rows in the worksheet "Properties". (See above.)

Values for  $\log K_{sw}$  and  $MW$  are retrieved from worksheet "Properties", using an INDEX-MATCH function.

"not used" appears when PRC name is left blank.

Type retained PRC fractions in the columns with header " $f_{obs}$ ", or use Copy + Paste Values. Blank cells are ignored in the calculations.

#### Block 4: Accumulated amounts

Block 4				
Accumulated amounts				
compound	$MW$	$\log K_{sw}$	$N$ (ng)	$N$ (ng)
phenanthrene	178.23	3.82	35.5	70.6
fluoranthene	202.25	4.28	672.4	441.9
pyrene	202.25	4.39	14.5	14.6
benzo[a]pyrene	252.31	5.26	8.3	16.6
PCB 28	257.54	5.25	1.5	1.5
PCB 52	291.99	5.52	4.9	3.8
PCB 101	326.43	5.99	6.3	14.7
PCB 118	326.43	6.11	49.2	3.9
PCB 153	360.88	6.45	409.7	459.0
PCB 180	395.32	6.76	162.0	79.9
4,4'-DDE	318.03	6.04	70.8	35.6

Select compound names of target analytes from the drop-down list.

Number of rows can be reduced by deleting rows, or increased by copy/pasting complete rows from the bottom downwards. Always keep the top row.

#### Block 5: Results

Run the solver add-in before inspecting the results (Far right on Data tab, Solver, Solve, OK). When Solver reports a convergence error, try an initial default value of  $\beta_M = 100$  in block 5.

Solver Parameters

Set Objective:

To:  Max  Min  Value Of:

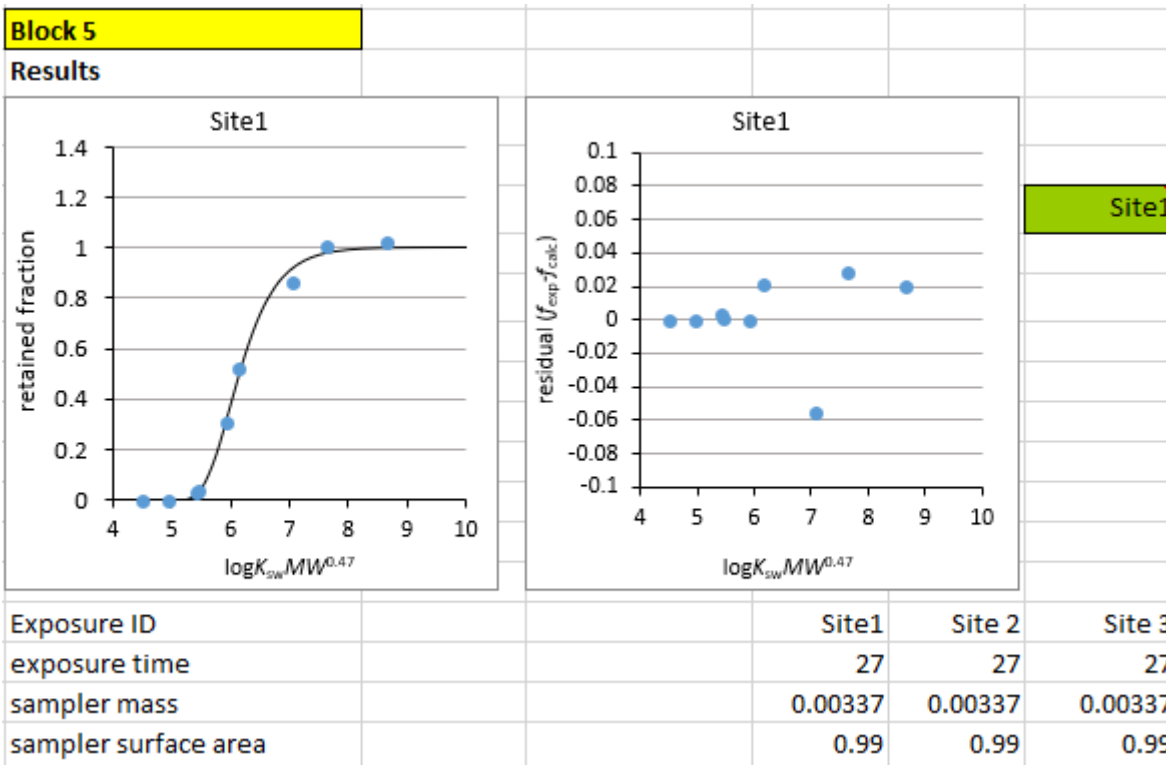
By Changing Variable Cells:

Subject to the Constraints:

Make Unconstrained Variables Non-Negative

Select a Solving Method:

Solving Method  
Select the GRG Nonlinear engine for Solver Problems that are smooth nonlinear. Select the LP Simplex engine for linear Solver Problems, and select the Evolutionary engine for Solver problems that are non-smooth.



At the top of the Results block inspect how well the model fits the retained PRC fractions.

Select the exposure of interest from the drop down box of the green cell.

The left plot shows retained PRC fractions and model fit. Right plot shows residual errors (difference between experimental and modelled fractions).

Vertical and horizontal scales can be modified as required.

Numerical results of the least squares estimation is shown below the graphs.

Model output		site 1	site 2
estimated $\beta_M$	$L d^{-1} g^{0.47} mol^{-0.47}$	119.1	112.4
S.E. in $\beta_M$	$L d^{-1} g^{0.47} mol^{-0.47}$	7.9	6.3
$R_{s\ 300}$	L/d	8.2	7.7
S.E. in $R_s$	L/d	0.5	0.4
$n$		8	8
$s_{fit}$	-	0.03	0.02
$R_{s\ 300} * t$	L	220	208
$R_{s\ 300}/A$	$L dm^{-2} d^{-1}$	8.2	7.8
smallest $f_{exp} - f_{calc}$	Vertical (Value) Axis	-0.06	-0.03
largest $f_{exp} - f_{calc}$	-	0.03	0.05

The estimated  $\beta_M$  and its standard error (S.E.) are shown in the first two rows. These values are used in the  $C_w$  calculations, but are difficult to interpret. Therefore the estimated  $R_s$  of a reference compound with  $MW = 300 g mol^{-1}$  and associated standard error are listed for reference.

$n$  is the number of PRC data that were used

$s_{fit}$  is the standard error of the model fit.

$R_{s,300} * t$  gives an indication of the equivalent water volume that is extracted for compounds that remained in the kinetic sampling stage.



$R_{s,300}/A$  gives an indication of the mass transfer coefficient of the water boundary layer. This value typically is in the range  $1 \text{ L dm}^{-2} \text{ d}^{-1}$  for quiescent waters and  $50 \text{ L dm}^{-2} \text{ d}^{-1}$  for very turbulent waters (flow velocities of several  $\text{m s}^{-1}$ ).

Smallest and largest residual errors are listed to help find the range that should be used for the residuals plot.

### Block 6: $C_w$ summary

Aqueous concentrations, exposure parameters, and model parameters are summarized in the rows below the model output.

Block 6				
Aqueous concentrations				
compound	MW	$\log K_{sw}$	$C_w$ (pg/L)	$C_w$ (pg/L)
phenanthrene	178.23	3.82	1592.6	3171.4
fluoranthene	202.25	4.28	10642.1	7024.5
pyrene	202.25	4.39	182.2	185.8
benzo[a]pyrene	252.31	5.26	41.8	88.0
PCB 28	257.54	5.25	7.9	8.0
PCB 52	291.99	5.52	24.4	20.0
PCB 101	326.43	5.99	30.6	75.9
PCB 118	326.43	6.11	238.3	20.0
PCB 153	360.88	6.45	2050.1	2431.7
PCB 180	395.32	6.76	841.5	439.7
4,4'-DDE	318.03	6.04	339.9	180.8

The output data from blocks 5 and 6 can be copied and pasted as values in another workbook, for reporting and further processing.

### Note on replication

Sampler replicates can be processed based on the PRC data and accumulated amount data for the individual samplers, but it is often better to apply a different pooling strategy. Absorbed amounts for replicates within the same exposure are usually highly similar, which indicates that the actual sampling rates are also similar. PRC based  $R_s$  estimates are usually more variable than accumulated amounts. This suggests that PRC data are preferably pooled, prior to the calculation of  $C_w$  for the individual samplers, as shown on next page.

## 3. Template validation

The template was tested using fabricated sampler data with zero noise (random exposure time, sampler thickness, area, sampling rate). Ratios of model output ( $\beta_M$ ,  $R_{s,300}$ ,  $C_w$ ) and imposed data were  $1.00000 \pm 0.00001$ .

Uncertainty estimates from the template were tested using fabricated sampler data with 5% random noise on the retained fractions. Estimates of  $\beta_M$  and its standard error were determined using present template and the nls method from R-project (R Development Core Team, 2019). Ratios of  $\beta_M$  and its standard error were  $1.00000 \pm 0.00001$ .

Block 2					
Exposure data				Replicate1	Replicate2
Exposure ID				27	27
exposure time	d			0.0034	0.0034
sampler mass	kg			0.99	0.99
sampler surface area	dm <sup>2</sup>				
Block 3					
Retained PRC fractions					
PRC name	MW	logK <sub>sw</sub>	f <sub>obs</sub>	f <sub>obs</sub>	
Fluorene-d10	176.20	3.44	0.000	0.000	
Anthracene-d10	188.20	3.88	0.000	0.000	
Pyrene-d10	212.25	4.34	0.032	0.032	
Chrysene-d12	240.36	4.80	0.311	0.311	
PCB 10	223.10	4.35	0.034	0.034	
PCB 30	257.54	5.01	0.520	0.520	
PCB 104	326.43	5.88	0.809	0.809	
PCB 145	360.88	6.44	1.007	1.007	
PCB 204	429.77	7.43	1.019	1.019	
Fluorene-d10	176.20	3.44	0.000	0.000	
Anthracene-d10	188.20	3.88	0.000	0.000	
Pyrene-d10	212.25	4.34	0.032	0.032	
Chrysene-d12	240.36	4.80	0.356	0.356	
PCB 10	223.10	4.35	0.039	0.039	
PCB 30	257.54	5.01	0.504	0.504	
PCB 104	326.43	5.88	0.941	0.941	
PCB 145	360.88	6.44	0.954	0.954	
PCB 204	429.77	7.43	1.043	1.043	

PRC data for Replicate 1

PRC data for Replicate 2

#### 4. Further support

This template comes with free online instructions for each purchase. Approximately 30 min should be sufficient. Contact [keesbooij@pasoc.eu](mailto:keesbooij@pasoc.eu) to set a date and time for this.

Contact [keesbooij@pasoc.eu](mailto:keesbooij@pasoc.eu) when the template needs to be tailored to your specific needs, when you need additional  $K_{sw}$  estimates, or when the template does not work as expected.

#### 5. Terms of use

Terms of use are summarised on the Readme tab of the template.

#### 6. Changes compared with previous version

The template was made more generally applicable to various types of samplers for hydrophobic compounds. Text of this manual was updated accordingly.

## 7. References

- Booij, K., 2021. Passive sampler exchange kinetics in large and small water volumes under mixed rate control by sorbent and water boundary layer. *Environmental Toxicology and Chemistry* 40, 1241–1254. <https://doi.org/10.1002/etc.4989>
- Booij, K., Hofmans, H.E., Fischer, C.V., van Weerlee, E.M., 2003. Temperature-dependent uptake rates of non-polar organic compounds by semipermeable membrane devices and low-density polyethylene membranes. *Environ.Sci.Technol.* 37, 361–366. <https://doi.org/10.1021/es025739i>
- Booij, K., Smedes, F., 2010. An improved method for estimating in situ sampling rates of nonpolar passive samplers. *Environ.Sci.Technol.* 44, 6789–6794. <https://doi.org/10.1021/es101321v>
- Booij, K., van Bommel, R., van Aken, H.M., van Haren, H., Brummer, G.J.A., Ridderinkhof, H., 2014. Passive sampling of nonpolar contaminants at three deep-ocean sites. *Environ.Pollut.* 195, 101–108. <https://doi.org/10.1016/j.envpol.2014.08.013>
- Ghosh, U., Driscoll, S.K., Burgess, R.M., Jonker, M.T.O., Reible, D., Gobas, F., Choi, Y.J., Apitz, S.E., Maruya, K.A., Gala, W.R., Mortimer, M., Beegan, C., 2014. Passive sampling methods for contaminated sediments: Practical guidance for selection, calibration, and implementation. *Integr.Environ.Assess.Manag.* 10, 210–223. <https://doi.org/10.1002/ieam.1507>
- Gilbert, D., Witt, G., Smedes, F., Mayer, P., 2016. Polymers as reference partitioning phase: polymer calibration for an analytically operational approach to quantify multimedia phase partitioning. *Anal. Chem.* 88, 5818–5826. <https://doi.org/10.1021/acs.analchem.6b00393>
- Grant, S., Schacht, V.J., Escher, B.I., Hawker, D.W., Gaus, C., 2016. Experimental solubility approach to determine PDMS–water partition constants and PDMS activity coefficients. *Environ. Sci. Technol.* 50, 3047–3054. <https://doi.org/10.1021/acs.est.5b04655>
- Huckins, J.N., Petty, J.D., Booij, K., 2006. *Monitors of organic chemicals in the environment: semipermeable membrane devices*. Springer, New York.
- Huckins, J.N., Petty, J.D., Lebo, J.A., Almeida, F.V., Booij, K., Alvarez, D.A., Cranor, W.L., Clark, R.C., Mogensen, B.B., 2002. Development of the permeability/performance reference compound approach for in situ calibration of semipermeable membrane devices. *Environ.Sci.Technol.* 36, 85–91. <https://doi.org/10.1021/es010991w>
- Jonker, M.T.O., van der Heijden, S.A., Kotte, M., Smedes, F., 2015. Quantifying the effects of temperature and salinity on partitioning of hydrophobic organic chemicals to silicone rubber passive samplers. *Environ.Sci.Technol.* 49, 6791–6799. <https://doi.org/10.1021/acs.est.5b00286>
- Kwon, J.H., Wuethrich, T., Mayer, P., Escher, B.I., 2007. Dynamic permeation method to determine partition coefficients of highly hydrophobic chemicals between poly(dimethylsiloxane) and water. *Anal.Chem.* 79, 6816–6822. <https://doi.org/10.1021/ac0710073>
- Lei, P., Zhu, J., Pan, K., Zhang, H., 2020. Sorption kinetics of parent and substituted PAHs for low-density polyethylene (LDPE): Determining their partition coefficients between LDPE and water (KLDPE) for passive sampling. *Journal of Environmental Sciences* 87, 349–360. <https://doi.org/10.1016/j.jes.2019.07.021>
- Lohmann, R., 2012. Critical review of low-density polyethylene's partitioning and diffusion coefficients for trace organic contaminants and implications for its use as a passive sampler. *Environ.Sci.Technol.* 46, 606–618. <https://doi.org/10.1021/es202702y>
- Muijs, B., Jonker, M.T.O., 2009. Temperature-dependent bioaccumulation of polycyclic aromatic hydrocarbons. *Environ.Sci.Technol.* 43, 4517–4523. <https://doi.org/10.1021/es803462y>
- Pintado-Herrera, M.G., Lara-Martín, P.A., González-Mazo, E., Allan, I.J., 2016. Determination of silicone rubber and low-density polyethylene diffusion and polymer/water partition coefficients

- for emerging contaminants. *Environ Toxicol Chem* 35, 2162–2172. <https://doi.org/10.1002/etc.3390>
- R Development Core Team, 2019. R: A language and environment for statistical computing. Version 3.6.2. R Foundation for Statistical Computing, Vienna, Austria.
- Reitsma, P.J., Adelman, D., Lohmann, R., 2013. Challenges of using polyethylene passive samplers to determine dissolved concentrations of parent and alkylated PAHs under cold and saline conditions. *Environ.Sci.Technol.* 47, 10429–10437. <https://doi.org/10.1021/es402528q>
- Schwarzenbach, R.P., Gschwend, P.M., Imboden, D.M., 2003. *Environmental Organic Chemistry*, 2nd ed. John Wiley & Sons, Hoboken, NJ, USA.
- Smedes, F., 2019. SSP silicone-, lipid- and SPMD-water partition coefficients of seventy hydrophobic organic contaminants and evaluation of the water concentration calculator for SPMD. *Chemosphere* 223, 748–757. <https://doi.org/10.1016/j.chemosphere.2019.01.164>
- Smedes, F., Beeltje, H., 2010. Silicone rubber-water partition coefficients for passive sampling. (No. 1201893- 000- BGS- 0001). Deltares, Utrecht.
- Smedes, F., Booij, K., 2012. Guidelines for passive sampling of hydrophobic contaminants in water using silicone rubber samplers. (No. ICES Techniques in Marine Environmental Sciences 52.). International Council for the Exploration of the Sea, Copenhagen. <https://dx.doi.org/10.17895/ices.pub.5077>.
- Smedes, F., Geertsma, R.W., van der Zande, T., Booij, K., 2009. Polymer-water partition coefficients of hydrophobic compounds for passive sampling: application of cosolvent models for validation. *Environ.Sci.Technol.* 43, 7047–7054. <https://doi.org/10.1021/es9009376>