S-Risk for the Walloon region - substance datasheet Polychlorinated Biphenyls (PCB): sum of the 7 congeners

M. Jailler, M. Paillet
October 2024

List of acronyms

ABS	Absorption factor
Al	Aluminum content
BCF	Bioconcentration factor
BTF	Biotransfer factor
Da	Diffusion coefficient in air
Dpe	Diffusion coefficient in polyethylene
Dpvc	Diffusion coefficient in PVC
Dw	Diffusion coefficient in water
FA	Factor used when calculating dermal absorption from water
Fe	Iron content
ISSeP	Institut Scientifique de Service Public
K_d	Sorption coëfficient soil-water
Koa	Distribution coefficient octanol-air
Koc	Distribution coefficient organic carbon-water
Kow	Distribution coefficient octanol-water
Kp	Dermale permeability coefficient
PAH	polycyclic aromatic hydrocarbons
PCB	Polychlorinated Biphenyls
Ptot	Total phosphorus content
TCA	Tolerable Concentration in Air
TDI	Tolerable Daily Intake
TGD	Technical Guidance Document

Introduction

Two major groups of PCBs can be distinguished based on their toxicological mode of action (INRS, 2019):

- Dioxin-like PCBs (PCB-DL), which can bind to the Aryl Hydrocarbon Receptor (AhR).
- Non-dioxin-like PCBs (PCB-NDL), which cannot bind to the AhR.

The most frequently detected congeners include PCBs 28, 52, 101, 118, 138, 153, and 180, collectively known as "indicator PCBs" and representing nearly 80% of PCBs found in the environment (INRS, 2019). Except for PCB 118 (a PCB-DL), all of these are PCB-NDLs. When PCB 118 is excluded, the remaining six are referred to as the "6 indicator PCBs" (ISSEP, 2020).

The default S-Risk parameters for PCBs were developed based on the sum of these 7 indicator PCBs (ISSEP, 2020), directly translated in French as PCB_Somme_7_Congeneres. These congeners were chosen for the following reasons (ATSDR, 2000; ISSEP, 2020):

- Toxicological data generally consider commercial mixtures of PCBs, making a simplified approach with reference toxicological values (RTVs) for congener mixtures the only viable option.
- In the environment, PCB congeners are always present as mixtures.
- Detailed analytical results for all congeners are rarely available in environmental investigations; results are typically presented as a total or blend of PCBs. RTVs are essential for assessing toxicity before a detailed characterization of the PCB profile is performed.

The proposal of TDI values for PCBi using a simplified approach is justified by the available toxicological data and the need for generic TDI values to interpret results for the sum of multiple congeners ("indicator PCBs"). However, due to varying toxicological properties among congeners, a more detailed toxicity and risk analysis should be conducted if (1) specific toxicological data for each congener are available, and (2) individual analytical data are available for each congener (ISSEP, 2020).

Congener profiles in environmental matrices differ based on emission source profiles, the matrix considered, and degradation processes. By measuring PCBi, the total amount of PCBs in a matrix can be estimated based on the relative proportion of these congeners in the PCB mixture (ISSEP, 2020).

The AwAC has adopted the German approach recommended by the "Länderarbeitsgemeinschaft Abfall (LAGA)", which suggests using a multiplication factor of 5 to extrapolate the total PCB concentration from the sum of the 6 PCBi for solid and liquid effluents. Thus, the concentration of the 6 PCBi identified in the matrix is multiplied by 5 to estimate the total PCB concentration (ISSEP, 2020).

For parameters linked to a single molecule (such as physico-chemical parameters), a worst-case approach was used. PCB 28 (2,4,4'-trichlorobiphenyl) was identified as the most critical congener among the seven evaluated.

PCB Somme 7 Congeneres

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	2,4,4'-trichlorobiphenyl	
Name S-Risk WAL		PCB_Somme_7_Congeneres	
CAS number	-	7012-37-5	
EC number	-	230-293-2	
Organic	-	Yes	
Dissociating	-	No	
Type Acid/Base	-	Base	
Acid constant - pKa	-	-	
Molar mass – M	g/mol	257.54	Mackay, D. (2006)
Temperature for water solubility - Ts	°C	20	Mackay, D. (2006)
Water solubility - S	mg/l	0.27	Mackay, D. (2006)
Temperature for P - Tp	°C	25	Mackay, D. (2006)
Vapour pressure - Pa	Pa	3.469E-2	Mackay, D. (2006)
Temperature for Henry coefficient - Th	°C	10	Mackay, D. (2006)
Henry coefficient - H	$Pa.m^3/mol$	1.906E+1	Mackay, D. (2006)
Organic carbon-water partition coefficient - Koc	dm^3/kg	4.039E+4	Calculated from Mackay, D. (2006)
Log Koc		4,610	Mackay, D. (2006)
Octanol-water partition coefficient - Kow	-	3.668E+5	Calculated from Mackay, D. (2006)
Log Kow		5.560	Mackay, D. (2006)
Permeation organic substance through PE pipe - Dpe	m^2/d	2E-7	RIVM. (2001)
Soil-water distribution coefficient - Kd	l/kg	Not relevant	

Exposure parameter	Unit	Value	Source
Dermal permeability coefficient - Kp	cm/h	0.269	Use model
Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0.14	Wester et al. (1993)
Fraction absorbed water - FA	-	0.8	Cornelis and al. (2017)

Plant	BCF plant type	Source
Potatoes	0.686	Cullen et al. (1996)
Potatoes		
Root and tuber vegetables	3.549	Cullen et al. (1996)
Carrots		
Salsify		
Other root vegetables (such as radish)		
Bulbous vegetables	3.549	Cullen et al. (1996)
Bulbous vegetables (such as onion)		
Leek		
Fruiting vegetables	1.514	Cullen et al. (1996)
Tomato		
Cucumber		
Other fruiting vegetables (such as peppers)		
Cabbages	14.20	Cullen et al. (1996)
Cabbage		
Cauliflower and broccoli		
Sprouts		
Leafy vegetables	14.20	Cullen et al. (1996)
Lettuce		
Lamb’s lettuce		
Endive		
Spinach		
Chicory		
Celery		
Legumes	1.514	Cullen et al. (1996)
Beans		
Peas		
Grasses	14.20	Cullen et al. (1996)
Grass		
Cereals	1.514	Cullen et al. (1996)
maize		

Animal parameter	Unit	Value	Source
Cow meat BTF	(mg/kg fw)/(mg/d)	1.075E-2	Use model (calculated value)
Cow liver BTF	(mg/kg fw)/(mg/d)	1.075E-2	Use model (calculated value)
Cow kidney BTF	(mg/kg fw)/(mg/d)	1.075E-2	Use model (calculated value)
Cow milk BTF	(mg/kg fw)/(mg/d)	2.910E-3	Use model (calculated value)
Sheep meat BTF	(mg/kg fw)/(mg/d)	1.075E-2	Use model (calculated value)

Limit value	Unit	Value	Source
Drinking water	µg/l		
Outdoor air	mg/m³		
Indoor air	mg/m³		

Reference toxicological value	Unit	Value	Source
Systemic effects threshold			
TCA inhalatory	mg/m³	5E-4	RIVM. (2001)
TDI oral	mg/(kg.d)	2E-5	WHO (2003)
TDI dermal	mg/(kg.d)	2E-5	Same as oral route
Averaging period		Child, adolescent, adult	
Systemic effects non-threshold			
Unit risk for inhalation	mg/m³	5.7E-1	OEHHA (2009)
Oral slope factor	$(mg/kg.d)^{-1}$	2E+0	OEHHA (2009)
Dermal slope factor	$(mg/kg.d)^{-1}$	2E+0	Same as oral route

References

ATSDR. (2000, November). *Toxicological profile for polychlorinated biphenyls (PCBs)*. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry.

Cullen, A. C., Vorhees, D. J., & Altshul, L. M. (1996). Influence of harbor contamination on the level and composition of polychlorinated biphenyls in produce in Greater New Bedford, Massachusetts. *Environmental Science & Technology, 30*(5), 1581-1588.

Cornelis, C., Standaert, A. & Willems, H. (2017) S-Risk Technical guidance document (version March 2017. Study accomplished under the authority of OVAM. https://srisk.be/sites/s-risk.be/files/SRisk%20model%20equations.pdf, pp. 174.

Lijzen, J. P. A., Rikken, M. G. J., Cornelis, C., & Swartjes, F. A. (2001, February). *Technical evaluation of the intervention values for soil/sediment and groundwater*. RIVM report 711701 023.

INRS. (2019, January). *Base de données Biotox - Fiche 194*. Institut National de Recherche et de Sécurité (INRS).

U.S. Environmental Protection Agency. (n.d.). *Integrated Risk Information System (IRIS) chemical assessment summary: Polychlorinated biphenyls (PCBs); CASRN 1336-36-3*. National Center for Environmental Assessment.

ISSEP. (2020, December 22). *Rapport de sélection de VTR par analyse simplifiée – PCBi* (rev. 12 September 2024). RP1-RAP-24-03079-EBO.

Länderarbeitsgemeinschaft Abfall (LAGA). (1998). *LAGA-Merkblatt: Entsorgung von PCB-haltigen Reststoffen und Abfällen 8375*. Berlin: Erich Schmidt Verlag.

Mackay, D. (2006). *Handbook of physical-chemical properties and environmental fate for organic chemicals*.

OEHHA. (2009). *Air Toxics Hot Spots Program Technical Support Document for Cancer Potencies: Appendix B. Chemical-specific summaries of the information used to derive unit risk and cancer potency values* (Updated 2011).

Wester, R. C., Maibach, H. I., Sedik, L., Melendres, J., & Wade, M. (1993). In vivo and in vitro percutaneous absorption and skin decontamination of arsenic from water and soil. *Fundamental and Applied Toxicology, 20*(3), 336-340.

WHO. (2003). *Polychlorinated biphenyls: Human health aspects*. https://iris.who.int/bitstream/handle/10665/42640/9241530553.pdf

Avenue Maurice Destenay 13 4000 Liège
Belgique
Tél. : +32 4 220 94 11
Fax : +32 4 221 40 43
communication@spaque.be · www.spaque.be