S-Risk for the Walloon region - substance datasheet: PFNA and PFHxS

M. Jailler
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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
Ptot	Total phosphorus content
TCA	Tolerable Concentration in Air
TDI	Tolerable Daily Intake
TGD	Technical Guidance Document

Introduction

As knowledge about environmental behaviour and toxicity of PFAS is moving fast, the chemicals encoded in S-RISK® WAL are indicated with the date, correlated with the date of the enforcement of the "Guidelines for PFAS" in Wallonia.

This specification allows to add these chemicals with updated data further without deleting the previous ones.

Due to surfactant properties of PFAS, some parameters are difficult to measure experimentally:

- the octanol-water coefficient **Kow** cannot be measured using current OECD methods. Kow is mandatory in S-Risk and has to be filled in anyway. For this, it can be calculated by EpiSuite even if EpiSuite is not recommended. To avoid using the Kow value in equations (equations to calculate Kp, Koc, BioConcentration Factors (BCF) and BioTransfer Factors (BTF)), **data of Kp, Koc, BCF and BTF must be encoded to obtain a correct result of risk**. The algorithms currently used for BCF and BTF (Trapp, Travis & Arms) are not applicable. Kow is entered in S-Risk but has not to be used in further calculations.

- the Henry constant **H** must be calculated by S-Risk, based on the vapour pressure and the solubility instead of encoding an experimental value.

- the PFAS are considered **"no dissociative**" because the Kd of dissociative substances is calculated from log Kow, which we want to avoid; for non-dissociative substances the Kd is calculated from the Koc.

For PFAS, some specificities are already taken account in the algorithm of the S-Risk® model core and need a specific key to consider them as PFAS. **All chemicals with a name starting by the 4 first letters "PFOA", "PFOS" or "PFAS" will be considered as a PFAS for the calculation**. It allows S-Risk to calculate the ingestion of vegetables with BioConcentration Factors (BCF) for soil/plant transfer expressed in different units.
As explained previously, BCF for soil/plant transfer must be encoded if the ingestion of vegetables pathway is selected (e.g. residential and agricultural exposure scenarios). As the transfer of PFAS is linked to the soil concentration, the experimental BCF are expressed in scientific literature with different units: **(mg/kg plant dm)/(mg/kg soil dm**) instead of (mg/kg dm)/(mg/m^3) for classic chemicals.

PFNA and PFHxS_dec2024

The data used to calculate the limit values in soil for PFNA and PFHxS in S-Risk® WAL were selected in May 2024 by SPAQUE and then validated by ISSeP.

PFNA and PFHxS are both non-volatile chemicals (Vp < 1 Pa).

Due to few data on soil/plant transfer, the maximal BCF value for a vegetable was selected, following the precautional principle. Only data could be checked (ratio of the vegetable concentration on the soil concentration) were used.

The Toxicity Reference Value (TRV) established by EFSA for oral route in 2020 for the sum of PFOA, PFOS, PFHxS and PFNA was selected. The calculation of the risk was done for the entire life (child + teenager + adult) and doesn't follow the VITO 's option (calculation only for adult). To use a TRV based on a sum of 4 chemicals in order to obtain separate threshold values for each PFAS is not correct, but this development was done before the updating of TRV expected in 2025.

PFNA-dec2024

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	Perfluorononanoic acid	Pubchem
Name S-Risk WAL	-	PFAS_PFNA_dec2024	
Molecular formula		$C_9HF_{17}O_2$	Pubchem
CAS number	-	375-95-1	Pubchem
EC number	-	206-801-3	Pubchem
Organic	-	Yes	
Dissociating	-	No	
Type Acid/Base	-	/	
Acid constant - pKa		Not applicable	Ssi 2 < pKa < 12
Molar mass – M	g/mol	464,08	Pubchem
Temperature for water solubility - Ts	°C	20	
Water solubility - S	mg/l	1299	CompTox
Temperature for P - Tp	°C	25	
Vapour pressure - Pa	Pa	0,66	Zhang (2020) cité dans PuChem
Temperature for Henry coefficient - Th	°C	25	
Henry coefficient - H	$Pa.m^3/mol$	0,2357	Calculated from H = (P x M) / S
Organic carbon-water partition coefficient - Koc	dm^3/kg	245,5	Higgins and Luthy (2006) cités dans ATSDR, US_EPA, RAIS
Log Koc		2,39	
Octanol-water partition coefficient - Kow	-	371,53	US-EPA, RAIS
Log Kow		2,57	
Permeation organic substance through PE pipe - Dpe	m^2/d		No data
Permeation organic substance through PVC pipe - Dpvc	m^2/d		No data
Soil-water distribution coefficient Kd	l/kg	Not relevant	

Exposure parameter	Unit	Value	Source

Dermal permeability coefficient - Kp	cm/h	$1,99.10^{-4}$	US-EPA – RAGS-E
Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0,1	RAIS et US-EPA RAGS-E
Fraction absorbed water - FA	-	1	

Plant	BCF plant	Source
Potatoes		
Potatoes	0,06	No experimental data – Value for PFOA (worst case)
Root and tuber vegetables		
Carrots	1,4	Lasee (2019). Maximal value in a sandy soil
Salsify	1,4	Highest value between radish and carrot
Other root vegetables (such as radish)	1,32	Blaine et al. (2014). Highest value between 0,98 and 1,32
Bulbous vegetables		
Bulbous vegetables (such as onion)	1,4	Highest value between radish and carrot
Leek	1,4	Highest value between radish and carrot
Fruiting vegetables		
Tomato	0,81	Blaine (2013) and Navarro (2017) : not detected in tomato Value for PFOA (worst case)
Cucumber	0,81	Highest value for fruiting vegetables
Other fruiting vegetables (such as peppers)	0,06	Moshfeghi (2015) – low confidence
Cabbages		
Cabbage	0,55	Value for PFOA (worst case)
Cauliflower and broccoli	0,55	Value for PFOA (worst case)
Sprouts	0,55	Value for PFOA (worst case)
Leafy vegetables		
Lettuce	2,85	Blaine et al. (2013) – Highest value between 0,77 and 2,85
Lamb's lettuce	2,85	= lettuce BCF
Endive	2,85	= lettuce BCF
Spinach	2,85	Navarro (2017) : not detected → lettuce BCF
Chicory	2,85	= lettuce BCF
Celery	0,68	Blaine et al. (2014). Highest value between 0,26 and 0,68
Legumes		
Beans	0,07	= peas BCF
Peas	0,07	Blaine et al. (2014). Highest value between 0,07 and limit of quantification

Grasses		
Grass	1,7	Lasee (2019). Worst case in a sandy soil
Cereals		
maize	0,16	Krippner (2015). Highest value between 0,12 and 0,16

Animal parameter	Unit	Value	Source
Cow meat BTF	(mg/kg fw)/(mg/d)	$3{,}019.10^{-2}$	Vestergren et al. (2013). Log BTF = -1,52
Cow liver BTF	(mg/kg fw)/(mg/d)	$1{,}010.10^{-1}$	calculated by SPAQUE from Vestergren et al. (2013)
Cow kidney BTF	(mg/kg fw)/(mg/d)	$8{,}853.10^{-6}$	Calculated by model
Cow milk BTF	(mg/kg fw)/(mg/d)	$1{,}548.10^{-2}$	Vestergren et al. (2013). Log BTF = -1,81
Sheep meat BTF	(mg/kg fw)/(mg/d)	$8{,}853.10^{-6}$	Calculated by model
Chicken - soil to egg BTF	(mg/kg fw)/(mg/d)		
Chicken - feed to egg BTF	(mg/kg fw)/(mg/d)		

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

Toxicological Reference value	Unit	Value	Source
Systemic effects threshold			
TCA inhalatory	mg/m³	$2{,}205.10^{-6}$	Route-to-route extrapolation – calculated by SPAQuE
TDI oral	mg/(kg.d)	$6{,}3.10^{-7}$	EFSA (2020) – TWI = 4,4 ng/kg.week for the sum of 4 PFAS : PFOA, PFOS, PFNA and PFHxS
TDI dermal	mg/(kg.d)	$6{,}3.10^{-7}$	= TDI oral
Systemic effects non-threshold			
Unit risk for inhalation	$(mg/m^3)^{-1}$		
Oral slope factor	$(mg/kg.d)^{-1}$		

Dermal slope factor	$(mg/kg.d)^{-1}$		

PFHxS-dec2024

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	Perfluorohexane sulfonic acid	Pubchem
Name S-Risk WAL	-	PFAS_PFHxS_dec2024	
Molecular formula		$C_6F_{13}SO_3H$	Pubchem
CAS number	-	355-46-4	Pubchem
EC number	-	206-587-1	Pubchem
Organic	-	Yes	
Dissociating	-	No	
Type Acid/Base	-	/	
Acid constant - pKa		Not applicable	Ssi 2 < pKa < 12
Molar mass – M	g/mol	400,12	Pubchem
Temperature for water solubility - Ts	°C	20	
Water solubility - S	mg/l	243	US-EPA (RSL), CompTox and RAIS
Temperature for P - Tp	°C	20	
Vapour pressure - Pa	Pa	$1{,}08.10^{-6}$	CompTox
Temperature for Henry coefficient - Th	°C	20	
Henry coefficient - H	$Pa.m^3/mol$	$1{,}78.10^{-6}$	Calculated from H = (P x M) / S
Organic carbon-water partition coefficient - Koc	dm^3/kg	190,54	Mac Guire (2014) cited in ATSDR
Log Koc		2,28	
Octanol-water partition coefficient - Kow	-	158,48	US-EPA (RSL), CompTox and RAIS
Log Kow		2,20	
Permeation organic substance through PE pipe - Dpe	m^2/d		No data
Permeation organic substance through PVC pipe - Dpvc	m^2/d		No data
Kd	l/kg	Not relevant	

Exposure parameter	Unit	Value	Source
Dermal permeability coefficient - Kp	cm/h	$2,58.10^{-4}$	US-EPA (RSL)- RAGS-E
Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0,1	RAIS – RAGS-E
Fraction absorbed water - FA	-	1	

Plant	BCF plant	Source
Potatoes		
Potatoes	0,01	Value for PFOS – no worst case
Root and tuber vegetables		
Carrots	1,1	Lasee (2019). Maximal value in a sandy soil
Salsify	2,06	Highest value in "root and tuber"
Other root vegetables (such as radish)	2,06	Blaine et al. (2014). Highest value between 0,85 and 2,06
Bulbous vegetables		
Bulbous vegetables (such as onion)	2,06	Highest value in "root and tuber"
Leek	2,06	Highest value in "root and tuber"
Fruiting vegetables		
Tomato	0,55	Blaine (2013)
Cucumber	0,55	Highest value in "fruiting"
Other fruiting vegetables (such as peppers)	0,09	Moshfeghi (2015) but low confidence
Cabbages		
Cabbage	2,06	Highest value in "root and tuber"
Cauliflower and broccoli	2,06	Highest value in "root and tuber"
Sprouts	2,06	Highest value in "root and tuber"
Leafy vegetables		
Lettuce	7,56	Blaine (2013). Highest value between 1,08 and 7,56
Lamb's lettuce	7,56	= lettuce BCF
Endive	7,56	= lettuce BCF
Spinach	7,56	= lettuce BCF
Chicory	7,56	= lettuce BCF
Celery	2,31	Blaine et al. (2014). Highest value between 0,07 and 2,31
Legumes		
Beans	0,17	= peas BCF
Peas	0,17	Blaine et al. (2014). Highest value between 0,17 and limit of quantification
Grasses		

Grass	12	Lasee (2019). Maximal value in a sandy soil
Cereals		
maize	0,85	Krippner (2015). Highest value between 0,84 and 0,85

Animal parameter	Unit	Value	Source
Cow meat BTF	(mg/kg fw)/(mg/d)	$6{,}885.10^{-3}$	Kowalczyk et al. (2013)
Cow liver BTF	(mg/kg fw)/(mg/d)	$2{,}192.10^{-2}$	Kowalczyk et al. (2013)
Cow kidney BTF	(mg/kg fw)/(mg/d)	$3{,}540.10^{-2}$	Kowalczyk et al. (2013)
Cow milk BTF	(mg/kg fw)/(mg/d)	$6{,}704.10^{-4}$	Kowalczyk et al. (2013)
Sheep meat BTF	(mg/kg fw)/(mg/d)	$3{,}681.10^{-6}$	Calculated by S-Risk
Chicken - soil to egg BTF	(mg/kg fw)/(mg/d)		
Chicken - feed to egg BTF	(mg/kg fw)/(mg/d)		

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

Toxicological Reference value	Unit	Value	Source
Systemic effects threshold			
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TDI oral	mg/(kg.d)	$6{,}3.10^{-7}$	EFSA (2020) – TWI = 4,4 ng/kg.week for the sum of 4 PFAS : PFOA, PFOS, PFNA and PFHxS
TDI dermal	mg/(kg.d)	$6{,}3.10^{-7}$	= TDI oral
Systemic effects non-threshold			
Unit risk for inhalation	$(mg/m^3)^{-1}$		
Oral slope factor	$(mg/kg.d)^{-1}$		
Dermal slope factor	$(mg/kg.d)^{-1}$		

References

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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