ANNEX A: PFOS SUBSTANCE SHEET

Parameter	Unit	Value	Source
Name		Perfluorooctane sulfonic acid	
CAS number		1763-23-1	
EC number		217-179-8	
Type		organic	
Dissociative		no[1]	
Acid constant (pKa)		-3.27	Brooke et al. (2004)
Molar mass	g/mol	500,126	
Water solubility	mg/l	370 (K-salt)[2]	OECD (2002)
Vapour pressure	Pa	$3.31.10^{-4}$ (K-salt) (20°C)	OECD (2002)
Henry coefficient	Pa m³/mol	-	Calculated in S-Risk
Log K_{ow}[1] K_{ow}	g/g	4.49 (calculated value)[3] 30902,95	EpiSuite
Log K_{oc} K_{oc}	dm³/kg	2.57 (anion) 371.54	Higgins and Luthy (2006)
Log K_{oa}	g/g	-[4]	optional in S-Risk
BCF	(mg/kg dm)/(mg/m³)	see table below	
Dpe	m²/d	1.10^{-7} (standard value)	Based on Vonk (1985) and Lijzen et al. (2011)
Dpvc	m²/d	1.10^{-10} (Dpe/1000)	Cornelis et al. (2017)
Diffusion for organic substance in air (Da)	m²/d	-	Calculated in S-Risk
Diffusion for organic substance in water (Dw)	m²/d	-	Calculated in S-Risk
Kp	[cm/h]	$9.5.10^{-7}$ (AFPO)	Washburn et al. (2005)
FA	-	1	Cornelis et al. (2017)
ABS dermal soil/dust	-	0	Xiao et al. (2015)
BTF beef	d/kg	0.071	Vestergren et al. (2013)

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[1] Entered in S-Risk but not used in further calculations

Parameter	Unit	Value	Source
BTF sheepmeat	d/kg	0.387	Kowalczyk et al 2012
BTF liver	d/kg	0.441	Vestergren *et al.* (2013)
BTF kidney	d/kg	1.201	(1) Kowalczyk *et al.* (2013)
BTF milk	d/kg	0.021	Vestergren *et al.* (2013)
BTF soil – egg	d/kg		
BTF food - egg	d/kg		
Carcinogenicity		Carc. 2	EG (2008)
Systemic effects threshold [5]			
TDI oral	mg/kg.d	2.10^{-5}	Preferred scenario US-EPA (2016)
TCA inhalatory	[mg/m³]	7.10^{-5}	calculated from TDI oral
TDI dermal	mg/kg.d	2.10^{-5}	= TDI oral
smoothing - ages		child, adolescent, adult	
Limit in air	mg/m³	-	
Limit in drinking water	mg/m³	0.1	EC (2018)
Crop standard	mg/kg fw		
Meat standard			
Beef	mg/kg fw		
Sheepmeat	mg/kg fw		
Liver	mg/kg fw		
Kidney	mg/kg fw		
Milk	mg/kg fw		
Butter	mg/kg fw		
Egg	mg/kg fw		
Dietary background all age groups including children	mg/kg day	$1.2.10^{-6}$ (1 - < 3 y)	Extrapolation based on EFSA (2012) Lower bound
		$1.2.10^{-6}$ (3 - < 6 y)	
		$1.08.10^{-6}$ (6 - < 10 y)	
		$0.513.10^{-6}$ (10 - < 15 y)	
		$0.562.10^{-6}$ (15 - < 21 y)	
		$0.634.10^{-6}$ (21 - < 31 y)	
		$0.875.10^{-6}$ ($\geq$ 31 y)	
Background potato	mg/kg fw	$3.60.10^{-6}$	EFSA (2012) LB
Background root vegetables	mg/kg fw	$9.50.10^{-6}$	EFSA (2012) LB

Parameter	Unit	Value	Source
Background bulbous vegetables (onion, etc.)	mg/kg fw	$2.20.10^{-6}$	EFSA (2012) LB
Background fruiting vegetables	mg/kg fw	$2.10.10^{-6}$	EFSA (2012) LB
Background cabbage	mg/kg fw	$1.20.10^{-6}$	EFSA (2012) LB
Background leafy vegetables	mg/kg fw	6.10^{-7}	EFSA (2012) LB
Background legumes	mg/kg fw	0	EFSA (2012) LB
Background beef	mg/kg fw	$8.60.10^{-6}$	EFSA (2012) LB
Background offal	mg/kg fw	$4.20.10^{-4}$	EFSA (2012) LB
Background milk	mg/kg fw	$9.00.10^{-7}$	EFSA (2012) LB
Background butter	mg/kg fw	$8.2.10^{-4}$	EFSA (2012) LB (Assimilated to *animal fat*)
Background eggs	mg/kg fw	$3.7.10^{-5}$	EFSA (2012) LB
Background outdoor air	mg/m³	$1.4.10^{-9}$	P50 value from Cornelis *et al.* (2009)
Background indoor air	mg/m³	$1.6.10^{-9}$	Jahnke *et al.* (2007b) in Cornelis *et al.* (2009)
Background drinking water	mg/m³	0	Assimilated to zero since it is included in the intake estimation of EFSA (2012)

[1] in S-Risk 'no' is entered because the Kd of dissociative substances is calculated from log K_{ow}, which we want to avoid; for non-dissociative substances the Kd is calculated from the K_{oc}

[2] The value of 370 mg/l is given in OECD (2002) with reference to a 3M report from 1999, without mention of temperature. The OECD test protocol for solubility (OECD test guideline 105) states that the test should preferably be carried out at 20 ± 0.5°C. As such, 20°C is used in S-Risk.

[3] Log K_{ow} is mandatory in S-Risk, and is used to calculate Kp, K_{oc}, and transfer factors, unless an experimental value is entered. Experimental values are available for these three parameters.

[4] Log K_{oa} is optional in S-Risk, which uses K_{oa} in the calculation of transfer to plants; as experimental data are available for this purpose, a K_{oa} value is not necessary.

(5) Due to the ongoing discussions on the new proposed TDI of EFSA, scenarios with 3 different sets of toxicological reference values will be calculated. The three sets are in the table below.

Toxicological reference value	Value	Unit	Reference
Set 1 (preference)			
TDI oral	2.10^{-5}	mg/kg/d	US-EPA (2016c)
TCA inhalation	7.10^{-5}	mg/m³	calculated from TDI oral
TDI dermal	2.10^{-5}	mg/kg/d	= TDI oral
Set 2			
TDI oral	$6.25.10^{-6}$	mg/kg/d	Zeilmaker et al. (2018)
TCA inhalation	$21.9.10^{-6}$	mg/m³	calculated from TDI oral
TDI dermal	$6.25.10^{-6}$	mg/kg/d	= TDI oral
Set 3			
TDI oral	$1.8.10^{-6}$	mg/kg/d	EFSA (2018c)
TCA inhalation	$6.3.10^{-6}$	mg/m³	calculated from TDI oral
TDI dermal	$1.8.10^{-6}$	mg/kg/d	= TDI oral

The RfD of US-EPA (2016c) of **20 ng/kg bw/d** is proposed as a toxicological reference value for the calculation of the soil remediation value based on the following arguments:

- experts recognise that the current standard of EFSA is too high
- the more stringent EFSA standard is still provisional
- the Dutch MTR is more protective than the current TDI of EFSA, but is likely to be reviewed when EFSA publishes its final (more stringent) TDI
- the MRL of ATSDR is still provisional
- the RfD is based on a long-term study
- the value of the RfD is the same as that of Australia and New Zealand

the derivations of US-EPA and Australia/New Zealand are recent

Plant	BCF or BCF model
potatoes	
potatoes	**0.01**
root and tuber vegetables	
carrots	**0.50**
salsify	0.44 (= average known root and tuber vegetables)
other root vegetables (such as radish)	**0.38**
bulbous vegetables	
bulbous vegetables (such as onion)	0.44 (= average known root and tuber vegetables)
leek	0.44 (= average known root and tuber vegetables)
fruiting vegetables	
tomato	**0.06**
cucumber	**0.07**
other fruiting vegetables (such as peppers)	0.065 (average known fruiting vegetables)
cabbages	
cabbage	0.44 (= average known root and tuber vegetables)
cauliflower and broccoli	0.44 (= average known root and tuber vegetables)
sprouts	0.44 (= average known root and tuber vegetables)
leafy vegetables	
lettuce	**0.56**
lamb's lettuce	0.56 (= lettuce)
endive	0.62 (average lettuce and celery)
spinach	**3.77**
chicory	0.62 (average lettuce and celery)
celery	**0.72**
legumes	
beans	0.03 (= peas)
peas	**0.03**
grasses	
grass	**0.048**
cereals	
maize	**0.003**

ANNEX B: PFOA SUBSTANCE SHEET

Parameter	Unit	Value	Source
Name		Perfluorooctanoic acid	
CAS number EC number		335-67-1 206-397-9	
Type		organic	
Dissociative		no[1]	
Acid constant (pKa)		2.8	Moody and Field (2000)
Molar mass	g/mol	414,07	
Water solubility	mg/l	$9.5.10^3$ (25°C)	ECHA (2014)
Vapour pressure	Pa	$1.7.10^{-2}$ (10°C)	Lijzen *et al.* (2018)
Henry coefficient	Pa m³/mol	-	Calculated in S-Risk
Log K_{ow}^2 K_{ow}	g/g	4.81 (calculated value)[2] 64565,42	EpiSuite
Log K_{oc} K_{oc}	dm³/kg	2.06 114.82	Higgins and Luthy (2006)
Log K_{oa}	g/g	-[3]	optional in S-Risk
BCF	(mg/kg dm)/(mg/m³)	See table below	
Dpe	m²/d	1.10^{-7} (standard value)	Vonk (1985); Lijzen *et al.* (2018)
Dpvc	m²/d	1.10^{-10} (Dpe/1000)	Cornelis *et al.* (2017)
Diffusion for organic substance in air (Da)	m²/d	-	Calculated in S-Risk
Diffusion for organic substance in water (Dw)	m²/d	-	Calculated in S-Risk
Kp	[cm/h]	$9.49.10^{-7}$	Fasano *et al.* (2005)
FA	-	1	Cornelis *et al.* (2017)
ABS dermal soil/dust	-	0	Xiao *et al.* (2015)
BTF beef	d/kg	$5,999.10^{-3}$	Vestergren, 2013 and Kowalczyk *et al.* (2013)
BTF sheepmeat	d/kg	$6,950.10^{-3}$	Vestergren, 2013 and Kowalczyk *et al.* (2013)
BTF liver	d/kg	$8,756.10^{-3}$	Vestergren, 2013 and Kowalczyk *et al.* (2013)

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[2] Entered in S-Risk but not used in further calculations

Parameter	Unit	Value	Source
BTF kidney	d/kg	$1,945.10^{-3}$	Vestergren, 2013 and Kowalczyk *et al.* (2013)
BTF milk	d/kg	$5,686.10^{-3}$	Vestergren, 2013 and Kowalczyk *et al.* (2013)
BTF soil – egg	d/kg		
BTF food - egg	d/kg		
Carcinogenicity		Carc. 2	EC (2008)
Systemic effects threshold [4]			
TDI oral	mg/kg.d	2.10^{-5}	US-EPA (2016)
TCA inhalatory	mg/m³	7.10^{-5}	calculated from TDI oral
TDI dermal	mg/kg.d	2.10^{-5}	= TDI oral
smoothing - ages		child, adolescent, adult	
Systemic effects without threshold			
Slope factor oral	(mg/kg/d)$^{-1}$	$0.07^{(5)}$	US-EPA (2016d)
Unit risk	(mg/m³)$^{-1}$	-	
Slope factor dermal	(mg/kg/d)$^{-1}$	-	
Smoothing duration		lifelong	
Limit in air	mg/m³	-	
Limit in drinking water	mg/m³	0.1	EC (2018)
Crop standard	mg/kg fw		
Meat standard			
Beef	mg/kg fw		
Sheepmeat	mg/kg fw		
Liver	mg/kg fw		
Kidney	mg/kg fw		
Milk	mg/kg fw		
Butter	mg/kg fw		
Egg	mg/kg fw		
Dietary background all age groups including children	mg/kg day	$2.20.10^{-7}$ (1 - < 3 y)	Extrapolation based on EFSA (2012) Lower bound
		$1.98.10^{-7}$ (3 - < 6 y)	
		$1.62.10^{-7}$ (6 - < 10 y)	
		$1.08.10^{-7}$ (10 - < 15 y)	
		$0.924.10^{-7}$ (15 - < 21 y)	
		$0.98.10^{-7}$ (21 - < 31 y)	
		$1.11.10^{-7}$ (≥ 31 y)	
Background potato	mg/kg fw	$9.00.10^{-7}$	EFSA (2012) LB

Parameter	Unit	Value	Source
Background root vegetables	mg/kg fw	$3.4.10^{-6}$	EFSA (2012) LB
Background bulbous vegetables (onion, etc.)	mg/kg fw	$2.2.10^{-6}$	EFSA (2012) LB
Background fruiting vegetables	mg/kg fw	$4.5.10^{-6}$	EFSA (2012) LB
Background cabbage	mg/kg fw	$1.9.10^{-6}$	EFSA (2012) LB
Background leafy vegetables	mg/kg fw	$6.2.10^{-6}$	EFSA (2012) LB
Background legumes	mg/kg fw	$2.5.10^{-5}$	EFSA (2012) LB
Background beef	mg/kg fw	$6.1.10^{-6}$	EFSA (2012) LB
Background offal	mg/kg fw	$3.4.10^{-5}$	EFSA (2012) LB
Background milk	mg/kg fw	0	EFSA (2012) LB
Background butter	mg/kg fw	$1.7.10^{-6}$	EFSA (2012) LB assimilated to *animal fat*
Background eggs	mg/kg fw	$8.8.10^{-5}$	EFSA (2012) LB
Background outdoor air	mg/m³	$8.90.10^{-9}$	Cornelis *et al.* (2009)
Background indoor air	mg/m³	$8.90.10^{-9}$	Assimilated to outdoor air
Background drinking water	mg/m³	0	Assimilated to 0 since it is included in the intake estimation of EFSA (2012)

[1] in S-Risk 'no' is entered because the Kd of dissociative substances is calculated from log K_{ow}, which we want to avoid; for non-dissociative substances the Kd is calculated from the K_{oc}

[2] Log K_{ow} is mandatory in S-Risk, and is used to calculate Kp, K_{oc}, and transfer factors, unless an experimental value is entered. Experimental values are available for these three parameters.

[3] Log K_{oa} is optional in S-Risk, which uses K_{oa} in the calculation of transfer to plants; as experimental data are available for this purpose, a K_{oa} value is not necessary.

[4] Due to the ongoing discussions on the new proposed TDI of EFSA, scenarios with 3 different sets of toxicological reference values will be calculated. The three sets are in the table below.

[5] The slope factor corresponds with a dose of $1.43.10^{-4}$ mg/kg bw/d or 143 ng/kg bw/d for an additional cancer risk of $1/10^5$. This value is higher than the toxicological reference value (20 ng/kg bw/d) used for the derivation of the soil remediation values. Hence a soil remediation value based on carcinogenic effects was not derived as it could be expected to be higher than for non-carcinogenic effects. This statement is in line with US-EPA who confirmed that the lifetime health advisory (2.10^{-5} mg/kg bw/d) based on non-cancer effects is protective for the cancer endpoint (US-EPA, 2016b).

Toxicological reference value	Value	Unit	Reference
Set 1 (preference)			
TDI oral	2.10^{-5}	mg/kg/d	US-EPA (2016c)

TCA inhalation	7.10^{-5}	mg/m³	calculated from TDI oral
TDI dermal	2.10^{-5}	mg/kg/d	= TDI oral
Set 2			
TDI oral	$12.5.10^{-6}$	mg/kg/d	Zeilmaker et al. (2016)
TCA inhalation	$43.8.10^{-6}$	mg/m³	calculated from TDI oral
TDI dermal	$12.5.10^{-6}$	mg/kg/d	= TDI oral
Set 3			
TDI oral	$0.8.10^{-6}$	mg/kg/d	EFSA (2018c)
TCA inhalation	$2.8.10^{-6}$	mg/m³	calculated from TDI oral
TDI dermal	$0.8.10^{-6}$	mg/kg/d	= TDI oral

The RfD of US-EPA (2016c) of **20 ng/kg bw/d** is proposed as a toxicological reference value for the calculation of the soil remediation value based on the following arguments:
- experts recognise that the current standard of EFSA is too high
- the more stringent EFSA standard is still provisional
- the Dutch MTR is more protective than the current TDI of EFSA, but is likely to be reviewed when EFSA publishes its final (more stringent) TDI
- the MRL of ATSDR is still provisional
- the RfD is based on a long-term study
- the value of the RfD is the same as that of Australia and New Zealand
  the derivations of US-EPA and Australia/New Zealand are recent

BCF values PFOA

Plant	BCF or BCF model
potatoes	
potatoes	**0.06**
root and tuber vegetables	
carrots	**0.39**
salsify	0.55 (average value of known root and tuber vegetables)
other root vegetables (such as radish)	**0.70**
bulbous vegetables	0.55 (= average known root and tuber vegetables)
bulbous vegetables (such as onion)	0.55 (= average known root and tuber vegetables)
leek	0.55 (= average known root and tuber vegetables)
fruiting vegetables	
tomato	**0.81**
cucumber	**0.82**
other fruiting vegetables (such as peppers)	0.81 (=tomato)
Cabbages	
Cabbage	0.55 (= average known root and tuber vegetables)
cauliflower and broccoli	0.55 (= average known root and tuber vegetables)
sprouts	0.55 (= average known root and tuber vegetables)
leafy vegetables	
Lettuce	**1.90**
lamb's lettuce	1.90 (=sla)
endive	1.06 (= average of all known leafy vegetables)
spinach	**0.87**
chicory	1.06 (= average of all known leafy vegetables)
celery	**0.42**
legumes	
beans	0.03 (= peas)
peas	**0.03**
Grasses	
Grass	**0.128**
Cereals	
Maize	**0.005**