Distribution: General

Final report

S-Risk substance data sheets – Part 1: metals and arsenic

C. Cornelis, J. Bierkens, A. Standaert

Study accomplished under the authority of OVAM
2016/MRG/R/0510

February 2017

VITO NV
Boeretang 200 - 2400 MOL - BELGIE
Tel. + 32 14 33 55 11 - Fax + 32 14 33 55 99
vito@vito.be - www.vito.be

BTW BE-0244.195.916 RPR (Turnhout)
Bank 375-1117354-90 ING
BE34 3751 1173 5490 - BBRUBEBB

2016/MRG/R/0510

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LIST OF ACRONYMS

ABS	Absorption factor
Al	Aluminum content
BCF	Bioconcentration factor
BTEXS	benzene, toluene, ethylbenzene, styrene
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
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
MTBE	methyl-t-butylether
OVAM	Openbare Vlaamse Afvalstoffenmaatschappij (Public Waste Agency of Flanders)
PAH	polycyclic aromatic hydrocarbons
Ptot	Total phosphorus content
SF	Slope Factor
TCA	Tolerable Concentration in Air
TDI	Tolerable Daily Intake
TDU	Tolerable Daily Uptake
OC	Organic Carbon
OM	Organic Matter

LIST OF MODIFICATIONS

17/12/2014	the reference of the Pb sheep BTF was corrected
20/01/2016	The soil-spinach BCF for arsenic was modified. The BCF resulted in a decrease of the arsenic concentration in the plant at increasing soil concentrations. This led to inconsistencies when using application I and III of S-Risk. The impact of the modified BCF on model results is minimal. The old BCF model: log BCF = -3.36 – 1.1 log As_{tot} + 0.99 log P_{tot}. The new BCF model: log BCF = -0.484 – 0.974 log As_{tot}.
17/08/2016	The CAS number for arsenic was corrected.
09/09/2016	The CAS number for zinc was corrected.
06/02/2017	Typos corrected.

INTRODUCTION

The substance data sheets summarise the data as available in S-Risk 1.0. The substance data sheets are a copy of those used for the calculation of the proposed soil clean-up values in Flanders. Following changes in model equations in S-Risk compared to the formerly used Vlier-Humaan model, some new parameter values had to be introduced. Also some supplementary options available in S-Risk required changes to the input data for which new values had to be collected. The most important changes are;

- **Dermal absorption**: Two new parameters are used that replace the formely used parameters to calculate dermal absorption, namely the fraction adsorbed for dermal uptake via soil and dust, and the dermal permeability coefficient for dermal uptake from water. The latter parameter is combined with a parameter FA.
- **Bioconcentration factors plants (BCF)**: For metals and arsenic very often either the BCF for maize or the BCF for grass was missing. In these cases the same BCF was used for maize and grass. Because this is incorrect, there is a need to search for additional BCFs.
- **Bioconcentration factors plants (BCF):** for organic compounds plant uptake in S-Risk can either be calculated starting from substance- and plant-specific characteristics or directly from BCF values expressed in mg/kg dm in the plant per mg/m^3 soil solution. For most organic substances plant uptake is calculated. For some organic substances however, BCF values reported in the original (Vlier-Humaan) data sheets had units of mg/kg dm in the plant per mg/kg dm in the soil, which are incompatible with the current S-Risk version. For these substances plant- and substance specific characteristics were used to calculate plant uptake. If so, this is mentioned in the data sheets.
- **Biotransfer factors animal products (BTF)**: S-Risk allows to specify BTF animal products by meat, milk, kidney and liver. For inorganic substances BTF values need to be filled in. The original data sheets only provided values for meat and milk. Lacking values were collected from De Raeymaecker et al. (2005). For organic substances model calculations are always used to obtain BTF values.
- **Biotransfer factors eggs (BTF):** S-Risk allows the user to calculate transfer to chicken eggs. This is a new feature as compared to Vlier-Humaan. However, using default settings in S-Risk this exposure route is not activated. For metals biotransfer factors to eggs have been collected and are included in the substance data sheets. For organic substances no BTF have been collected and their value has been equaled to zero. When the exposure route to eggs is activated in S-Risk the user should enter appropriate BTF values.
- **Toxicity data**: The toxicity data in S-Risk are copied from the original substance data sheets. In contrast to Vlier-Humaan, where calculations were only possible for systemic effects and either carcinogenic or non-carcinogenic effects, S-Risk allows to make calculations for several endpoints simultaneously. As a consequence, the toxicity data in the current substance data sheets are sometimes more extensive than in the former ones.
- **Background exposure and background concentrations**: Vlier-Humaan did only allow to enter one value for background exposure (be it depending on the type of land use) via food. In S-Risk it is possible to enter age-dependent background exposure via food. Default ratios are most often used for age-dependency (according the the ratio's specified in the TGD). Differences between land-uses are taken into account based on the background concentrations for food that have been entered. S-Risk also separately calculates background exposure via drinking water.

- **Limit values for food**: For some substances calculated concentrations in food stuffs have to comply with existing standards. With this in mind recent legislation has been scrutinised and obsolete values were replaced by more recent ones when appropriate.

The existing information, which was copied in S-Risk is based on the following original substance data sheets:

- Heavy metals: OVAM (2009c) and (OVAM, 2009d) with accompanying spreadsheet;
- BTEXS: OVAM (2009a);
- Chlorinated aliphatic substances: OVAM (2004) for 1,1,1-trichloroethane, 1,1,2-trichloroethane, 1,1-dichloroethane, cis-1,2-dichloroethene, trans-1,2-dichloroethene, dichloromethane, tetrachloroethene, tetrachloromethane, trichloroethene; OVAM (2009b) for 1,2-dichloroethane, vinyl chloride, trichloromethane (chloroform);
- Chloro-aromatics: OVAM (2004); OVAM (2009b) for hexachloro-benzene;
- PAHs: OVAM (2003a) for PAHs; OVAM (2005a) for changes in the evaluation criteria for for benzo(a)pyrene and dibenz(a,h)antracene;
- Cyanides: OVAM (2004);
- Trimethylbenzenes: OVAM (2003b);
- Chlorophenols: OVAM (2005b)
- Hexane, heptane, octane: OVAM (2004);
- MTBE: OVAM (2003a)

Details on the new information is always available in the report discussing the calculation of clean-up values with S-Risk (Cornelis, Bierkens, and Standaert, 2013a). Newly added or modified information compared to the original data sheets is clearly indicated in the S-Risk substance data sheets.

The substance data sheets consist of 6 documents:

- **Part 1: Substance data sheets metals and arsenic**
- Part 2: Substance data sheets benzene, toluene, ethylbenzene, xylenes, styrene and trimethylbenzenes
- Part 3: Substance data sheets chlorinated aliphatic substances, chloro benzenes and chlorophenols
- Part 4: Substance data sheets polycylic aromatic hydrocarbons
- Part 5: Substance data sheets alkanes, MTBE and cyanides
- Part 6: Substance data sheets total petroleum hydrocarbons.

CHAPTER 1 SUBSTANCE DATA SHEET HEAVY METALS

Data on substances that do not derive from the former substance data sheets are indicated with **N**, accompanied with some explanation if appropriate. Detailed information on all new entries is given in Cornelis et al. (2013a).

The plant uptake factors for *copper, mercury and nickel* were derived for non-enriched soils. For enriched soils these BCF are divided by a certain factor. The distinction between enriched and non-enriched soils is derived by multiplying the background value by 4. The background values are the values included in the version of Vlarebo preceding the 2008 version.

1.1. Arsenic

Parameter	Unit	Value	Source
CAS nr.		7440-38-2	
Type		inorganic	
Molecular weight	g/mol	74.9	Geometric mean
Solubility	mg/l	-	
Vapour pressure	Pa	0	
Henry coefficient	Pa m³/mol	0	
Kd	dm³/kg	log K_d = 1.68 + (1.26 x log (%clay)) [a)]	Based on data from Smolders et al. (2000)
BCF		[b)]	Ruttens (2005)
Dpe	m²/d	0	
Dpvc	m²/d	0	
Diffusion coefficient air (Da)	m²/d	calculated	
Diffusion coefficient water (Dw)	m²/d	calculated	
Kp	[cm/h]	$1.00x10^{-3}$	US-EPA (2004b)
FA	-	1	
ABS dermal soil/dust	-	$3.00x10^{-2}$	Wester et al. (1993) in US-EPA (2004a)
BTF beef	d/kg	$1.36x10^{-3}$	De Raeymaecker et al. (2006)
BTF mutton	d/kg	$2.50x10^{-3}$	Beresford et al. (2001)
BTF liver	d/kg	$4.20x10^{-3}$	Crout et al. (2004)
BTF kidney	d/kg	$4.90x10^{-3}$	Crout et al. (2004)
BTF milk	d/kg	$1.00x10^{-4}$	De Raeymaecker et al. (2006)
BTF soil – egg	d/kg	$4.60x10^{-1}$	same value as BTF feed-egg
BTF feed - egg	d/kg	$4.60x10^{-1}$	Sheppard et al. (2010)
Carcinogenicity		1 A 1	IARC (1987) US-EPA, (2002) EC (2001)
Systemic effects threshold			
TDI oral	mg/kg.d	$2x10^{-3}$	JECFA (1989a)
TCA inhalation [c)]	mg/m³	$1.3x10^{-5}$	Highest value proposed in EC (2001); higher than European target value for air quality (6 ng/m³)
TDI dermal	mg/kg.d	$2x10^{-3}$	same as oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m³	$1.30x10^{-5}$	Highest value proposed in EC (2001); higher than European target value for air quality (6 ng/m³)
Limit value in drinking water	mg/m³	10	WHO, (1993); Vl. Reg. (2003)

Parameter	Unit	Value	Source
Limit value in plants	mg/kg vg	Grass 0.8 Maize 0.56	Belgisch Staatsblad ("Ministerieel Besluit van 12 februari 19991 betreffende de handel en het gebruik van producten die bedoeld zijn voor het voederen van dieren, en wijzigingen," 1999) and modifications, adjusted values for dry matter
Limit value in meat			
Beef	mg/kg vg	-	
Mutton	mg/kg vg	-	
Liver	mg/kg vg	-	
Kidney	mg/kg vg	-	
Milk	mg/kg vg	-	
Butter	mg/kg vg	-	
Egg	mg/kg vg	-	
Dietary background adults	mg/kg dag	$2.58x10^{-4}$	Deelstra et al. (1996)
Dietary background children	mg/kg.dag	relative with regard to adultscfr. TGD	Cornelis et al. (2013b)
Background potatoes	mg/kg vg	0.002	MAFF (1999)
Background root crops	mg/kg vg	0.002	MAFF (1999)
Background bulbous plants (onion …)	mg/kg vg	0.002	MAFF (1999)
Background fruit vegetables	mg/kg vg	0.005	MAFF (1999)
Background cabbage	mg/kg vg	0.005	MAFF (1999)
Background leafy vegetables	mg/kg vg	0.003	MAFF (1999)
Background legume	mg/kg vg	0.005	MAFF (1999)
Background beef	mg/kg vg	0.003	MAFF (1999)
Background offal	mg/kg vg	0.004	MAFF (1999)
Background milk	mg/kg vg	0.0004	MAFF (1999)
Background butter	mg/kg vg	0.003	MAFF (1999)
Background eggs	mg/kg vg	0.0009	MAFF (1999)
Background outdoor air	mg/m^3	$4.80x10^{-6}$	VMM (2004) (average)
Background indoor air	mg/m^3	$4.80x10^{-6}$	= outdoor air
Background drinking water	mg/m^3	1.5	VMM (2006) (average of mean values at the tap)

a) Background information on the choice of the partition coefficient K_d can be found in Smolders et al. (2000).
Because the purpose was to derive a partition coefficient both for calculating soil intervention values and leaching standards, the Kd relationship used for remediation value calculations deviated from the on proposed in the report:
$\log K_d = 1.68 + (1.26 \times \log(\%clay))$ $R^2 = 0.49$
The K_d calculated for a standard soil (%clay: 10) equals 871 l/kg.

b) The choice of BCFs is based on Ruttens (2005). Available BCF regression models from this report as well as the rules that apply to assign BCF values to crops for which no BCF exist (equalisation rules) are summarized below (see table). As no BCF values are available for salsify, paprika and cabbage from the background report on proposed soil remediation values, we defined additional equalisation rules for these crops.

Plant species	BCF or BCF-model	
potatoes		
potatoes	0.003	Versluijs en Otte (2001)
root and tuberous crops		
carrots	log BCF = 0.57 - (0.66 x log As_{tot}) - (0.49 x log Fe)	
salsify	log BCF = 0.57 - (0.66 x log As_{tot}) - (0.49 x log Fe)	equal to carrots
Other root crops (e.g. radish)	0.12	potato * 40
bulbous crops		
bulbous crops (e.g. onion)	0.0163	average leafy vegetables/2 (for standard soil)
leek	log BCF = -3.05 – (0.54 x log As_{tot}) + (0.73 x log Al)	
fruit vegetables	0.003	
tomato	0.003	
cucumber	0.003	equal to potato
Other fruit vegetables (e.g. paprika)	0.003	equal to potato
cabbages	0.011	equal to Brusssels sprouts
cabbage		
cauliflower and broccoli	0.003	equal to potato
Brussels sprouts	0.011	average leafy vegetables/3 (standard soil)
leafy crops		
Lettuce	log BCF = -0.31 –(0.73 x log As_{tot})	
lamb's lettuce	0.033	average leafy vegetables
endive	0.033	average leafy vegetables
spinach	log BCF = -0.484 - (0.974 x log As_{tot})	modified 20/01/2016
chicory	0.011	average leafy vegetables/3
celery	log BCF = 1.08 - (0.54 x log As_{tot}) - (0.56 x log Fe)	
legume		
beans	0.003	equal to potato
peas	0.003	equal to potato
grasses		
grass	0.27	Van Wezel (2003)
cereals		
maize	0.27	equal to grass

[c] In the original substance data sheets the reference value for inhalation is expressed in units of mg/kg.d. In contrast the reference value used in S-Risk is expressed in units of mg/m^3. Conversion is done by multiplying the value in mg/kg.d by a value for the body weight of 70 Kg and dividing it by a value for the respiratory rate of 20 m^3/d. Although for the calculation of the soil standards arsenic is considered non-carcinogenic via the oral route and carcinogenic with threshold via the inhalation route (clearly different endpoints), the risk indexes were nevertheless summed. This was maintained in S-Risk.

1.2. Cadmium

Parameter	Unit	Value	Source
CAS nr.		7440-43-9	
Type		inorganic	
Molecular weight	g/mol	112.4	Geometric mean
Solubility	mg/l	-	
Vapour pressure	Pa	0	
Henry coefficient	Pa m³/mol	0	
Kd	dm³/kg	log K_d = -0.19 + (0.46 x pH) [a]	Smolders et al. (2000)
BCF		[b]	Smolders (2006)
Dpe	m²/d	0	
Dpvc	m²/d	0	
Diffusion coefficient air (Da)	m²/d	calculated	
Diffusion coefficient water (Dw)	m²/d	calculated	
Kp	[cm/h]	1.00×10^{-3}	US-EPA (2004b)
FA	-	1	
ABS dermal soil/dust	-	1.00×10^{-3}	Wester et al. (1992) in US-EPA (2004a)
BTF beef	d/kg	1.36×10^{-4}	De Raeymaecker et al. (2005)
BTF mutton	d/kg	2.20×10^{-2}	Morgan (1991)
BTF liver	d/kg	5.40×10^{-2}	Crout et al. (2004)
BTF kidney	d/kg	5.20×10^{-3}	Crout et al. (2004)
BTF milk	d/kg	1.90×10^{-6}	De Raeymaecker et al. (2005)
BTF soil – egg	d/kg	6.70×10^{-2}	same as feed-egg
BTF feed - egg	d/kg	6.70×10^{-2}	Sheppard et al. (2010)
Carcinogenicity		1	IARC (1993a, 1993b)
		B1	US-EPA (1998b)
		2	EC (2001) (cadmium chloride, oxide and sulphate)
		3	EC (2001) (cadmium sulphide)
Systemic effects threshold			
TDI oral	mg/kg.d	1.1×10^{-3}	JECFA (1989a, 1989b, 2001, 2004)
TCA inhalation [c]	mg/m³	5×10^{-6}	WHO (2000); EC (2001)
TDI dermal	mg/kg.d	5.5×10^{-5}	from oral TDI with oral absorption factor of 0.05
averaging period		lifelong	changed as compared to Vlier-Humaan because of effect after cumulative exposure [d]
Limit value in air	mg/m³	5.00×10^{-6}	EC (2001)
Limit value in drinking water	mg/m³	3	WHO (1993, 1996)

Parameter	Unit	Value	Source
Limit value in plants	mg/kg vg	Potatoes 0.1 Root crops 0.1 Bulbous plants 0.05 Fruit vegetables 0.05 Cabbage 0.05 Leafy vegetables 0.2 Legume 0.05 Grass 0.4 Mais 0.2	EC 1881/2006 ("Verordening 1881/2006 van de Commissie van 19 december 2006 tot vaststelling van de maximumgehalten aan bepaalde verontreinigingen in levensmiddelen," 2006) for food; 2002/32/EG (2002) for feed (grass, mais); : different values for dry matter feed; more vegetables
Limit value in meat			EC 1881/2006 ("Verordening 1881/2006 van de Commissie van 19 december 2006 tot vaststelling van de maximumgehalten aan bepaalde verontreinigingen in levensmiddelen," 2006) voor voeding
Beef	mg/kg vg	0.05	
Mutton	mg/kg vg	0.05	
Liver	mg/kg vg	0.5	
Kidney	mg/kg vg	1	
Milk	mg/kg vg	-	limit did exist in previous legislation
Butter	mg/kg vg	-	
Egg	mg/kg vg	-	
Background food adults	mg/kg dag	$2.33x10^{-4}$	Deelstra et al. (1996)
Background food children	mg/kg.dag	relative with regard to adults cfr. TGD	Cornelis et al. (2013b)
Background potato	mg/kg vg	0.036	MAFF (1999)
Background root crops	mg/kg vg	0.036	MAFF (1999)
Background bulbous plants (onion …)	mg/kg vg	0.036	MAFF (1999)
Background fruit vegetables	mg/kg vg	0.013	MAFF (1999)
Background cabbage	mg/kg vg	0.013	MAFF (1999)
Background leafy vegetables	mg/kg vg	0.033	MAFF (1999)
Background legume	mg/kg vg	0.013	MAFF (1999)
Background beef	mg/kg vg	0.006	MAFF (1999)
Background offal	mg/kg vg	0.094	MAFF (1999)
Background milk	mg/kg vg	0.0006	MAFF (1999)
Background butter	mg/kg vg	0.006	MAFF (1999)
Background eggs	mg/kg vg	0.003	MAFF (1999)
Background outdoor air	mg/m^3	$1.60x10^{-6}$	VMM (2004)
Background indoor air	mg/m^3	$1.60x10^{-6}$	= outdoor air
Background drinking water	mg/m^3	0.25	VMM (2006) (average of mean values at the tap)

[a] For the conversion of the K_d value of Cd as a function of pH($CaCl_2$, 0.01 M) the following equation is used (R^2 = 0.73): log K_d = -0.19 + (0.46 x pH). In this way a k_d value of 372 l/kg is

calculated at pH = 6. A different conversion formula was derived based on pH($CaCl_2$, 0.01 M) and CEC (R^2 = 0.79):

$\log K_d = -0.13 + (0.43 \times pH) + (0.26 \times \log CEC)$.

b) The choice of BCFs is based on Smolders (2006). Available BCF regression models from this report as well as the rules that apply to assign BCF values to crops for which no BCF exists (equalisation rules) are summarized below (see table). As paprika, cabbage and maize were not included in the background information to the guidelines on the derivation of soil remediation values for heavy metals, we defined additional equalisation rules for these crops.

Plant species	BCF orBCF-model	
potatoes		
potatoes	Log BCF = -0.5 – 0.05 pH-KCl – 0.73 log Cd_{soil}	Smolders (2006)
root- and tuberous crops		
carrots	Log BCF = 0.43 – 0.12 pH-KCl – 0.51 log Cd_{soil}	Smolders (2006)
salsify	Log BCF = 1.4 – 0.32 pH-KCl – 0.58 log Cd_{soil}	Smolders (2006)
Other root crops (e.g. radish)	0.271	potato (at background value soil *4, pH6)*4
bulbous crops		
bulbous crops (e.g. onion)	0.294	leek (at background value soil *4, pH6)
leek	Log BCF = 1.18 – 0.25 pH-KCl – 0.42 log Cd_{soil}	Smolders (2006)
fruit vegetables	Log BCF = -0.16 – 0.06 pH-KCl – 0.66 log Cd_{soil}	= Smolders (2006) voor tomaten
tomato	Log BCF = -0.16 – 0.06 pH-KCl – 0.66 log Cd_{soil}	Smolders (2006)
cucumber	Log BCF = -0.86 – 0.26 log Cd_{soil}	Smolders (2006)
Other fruit vegetables (e.g. paprika)		
cabbages	0.023	= Brussels sprouts
cabbage		
cauliflower and broccoli	0.068	potato (at background value soil *4, pH6)
Brussels sprouts	0.023	potato (at background value soil *4, pH6)/3
leafy crops		
Lettuce	Log BCF = 1.06 – 0.14 pH-KCl – 0.4 log Cd_{soil}	Smolders (2006)
lamb's lettuce	1.042	= Lettuce (at background value soil *4, pH6)
endive	Log BCF = 1.99 – 0.32 pH-KCl – 0.42 log Cd_{soil}	Smolders (2006)
spinach	Log BCF = 0.53 – 0.06 pH-KCl – 0.37 log Cd_{soil}	Smolders (2006)
Chicory	0.326	= average value leafy vegetables (at background value soil *4, pH6)/3
celery	Log BCF = 1.07 – 0.13 pH-KCl – 0.43 log Cd_{soil}	Smolders (2006)
legume		

Plant species	BCF orBCF-model	
beans	Log BCF = 0.43 – 0.34 pH-KCl + 0.24 log Cd_{soil}	Smolders (2006)
peas	0.032	= beans (at background value soil*4, pH6)
grasses		
grass	Log BCF = -0.33 – 0.08 pH-KCl – 0.78 log Cd_{soil}	Smolders (2006)
cereals		
maize	Log BCF = -0.33 – 0.08 pH-KCl – 0.78 log Cd_{soil}	= grass

c) In the original substance data sheets the reference value for inhalation is expressed in units of mg/kg.d. In contrast the reference value used in S-Risk is expressed in units of mg/m^3. Conversion is done by multiplying the value in mg/kg.d by a value for the body weight of 70 Kg and dividing it by a value for the respiratory rate of 20 m^3/d.

d) For the derivation of soil standards for Cd the default approach was applied whereby a separate risk index was calculated for children and adults. Due to the higher value for background exposure of children this yields already high risk indices at background levels. Therefore it was decided, also because of the toxic mode of action of Cd, to average out life-long exposure for the S-Risk calculations. Further evaluation of the toxicological reference value is however required

1.3. CHROMIUM (III)

Parameter	Unit	Value	Source
CAS nr.		7440-47-3	
Type		inorganic	
Molecular weight	g/mol	52	
Solubility	mg/l	-	
Vapour pressure	Pa	0	
Henry coefficient	Pa m³/mol	0	
Kd	dm³/kg	$\log K_d = 2.25 + (0.28 \times pH\text{-}CaCl_2)$	Smolders et al. (2000)
BCF		a)	Ruttens (2005)
Dpe	m²/d	0	
Dpvc	m²/d	0	
Diffusion coefficient air (Da)	m²/d	calculated	
Diffusion coefficient water (Dw)	m²/d	calculated	
Kp	[cm/h]	1.00×10^{-3}	US-EPA (2004b)
FA	-	1	
ABS dermal soil/dust	-	0	dermal contact = mainly local effect
BTF beef	d/kg	4.48×10^{-3}	De Raeymaecker et al. (2006)
BTF mutton	d/kg	4.48×10^{-3}	= beef
BTF liver	d/kg	1.80×10^{-3}	Stevens (1992)
BTF kidney	d/kg	1.60×10^{-4}	Stevens (1992)
BTF milk	d/kg	2.00×10^{-4}	De Raeymaecker et al. (2006)
BTF soil – eggi	d/kg	3.30×10^{-2}	= feed - egg
BTF feed - eggi	d/kg	3.30×10^{-2}	Sheppard et al. (2010)
Carcinogenicity		3 D	IARC (1990a) US-EPA (1998e)
Systemic effects threshold			
TDI oral	mg/kg.d	3×10^{-3}	ATSDR (2000)
TCA inhalation[b)]	mg/m³	1.05×10^{-2}	calculated from oral value
TDI dermal	mg/kg.d	3.9×10^{-5}	from oral TDI with oral absorption factor 0.013
averaging period		child, adolescent, adult	
Limit value in air	mg/m³	1.05×10^{-2}	calculated from oral value
Limit value in drinking water	mg/m³	50	WHO (WHO, 1996); EC (1998)
Limit value in plants	mg/kg vg	-	
Limit value in meat			
Beef	mg/kg vg	-	
Mutton	mg/kg vg	-	
Liver	mg/kg vg	-	
Kidney	mg/kg vg	-	
Milk	mg/kg vg	-	
Butter	mg/kg vg	-	
Egg	mg/kg vg	-	
Background food adults	mg/kg dag	5.10×10^{-4}	Deelstra et al. (1996)

Parameter	Unit	Value	Source
Background food children	mg/kg.dag	relative with regard to adults cfr. TGD	Cornelis et al. (2013b)
Background potato	mg/kg vg	0.04	MAFF (1999)
Background root crops	mg/kg vg	0.04	MAFF (1999)
Background bulbous plants (.onion …)	mg/kg vg	0.04	MAFF (1999)
Background fruit vegetables	mg/kg vg	0.04	MAFF (1999)
Background cabbage	mg/kg vg	0.04	MAFF (1999)
Background leafy vegetables	mg/kg vg	0.02	MAFF (1999)
Background legume	mg/kg vg	0.04	MAFF (1999)
Background beef	mg/kg vg	0.09	MAFF (1999)
Background offal	mg/kg vg	0.08	MAFF (1999)
Background milk	mg/kg vg	0.01	MAFF (1999)
Background butter	mg/kg vg	0.17	MAFF (1999)
Background eggs	mg/kg vg	0.04	MAFF (1999)
Background outdoor air	mg/m³	3.90×10^{-6}	VMM (2004)
Background indoor air	mg/m³	3.90×10^{-6}	= outdoor air
Background drinking water	mg/m³	1.00	VMM (2006)

([a]) The choice of BCFs is based on Ruttens (2005). These BCF were derived for total chromium but are used for both Cr(III) and Cr(VI). Calculated and estimated BCF values for the crops in the food package are shown in the table below. As salsify, parsnip, paprika, cabbage and maize were not included in the background information to the guidelines on the derivation of soil standards for heavy metals, we defined additional equalisation rules for these crops.

Plant species	BCF or BCF-model	
potatoes		
potatoes	0.019	
root- and tuberous crops	0.003	=carrot
carrots	0.003	
salsify		
Other root crops (e.g. radish)	0.019	= potato
bulbous crops		
bulbous crops (e.g. onion)	0.0004	
leek	0.0004	= onion
fruit vegetables		= tomato
tomato	0.0015	
cucumber	0.0015	= tomato
Other fruit vegetables (e.g. paprika)		
cabbages	0.019	= potato
cabbage		
cauliflower and broccoli		
Brussels sprouts		
leafy crops		
Lettuce	0.004	
lamb's lettuce	0.04	= average leafy vegetables from Ruttens (2005)
endive	0.04	= average leafy vegetables from Ruttens (2005)

Plant species	BCF or BCF-model	
spinach	0.04	= average leafy vegetables from Ruttens (2005)
Chicory	0.04	= average leafy vegetables from Ruttens (2005)
celery	0.04	= average leafy vegetables from Ruttens (2005)
legume		
beans	0.003	
peas	0.003	= beans
grasses		
grass	0.052	
cereals		
maize	0.052	= grass

b) In the original substance data sheets the reference value for inhalation is expressed in units of mg/kg.d. In contrast the reference value used in S-Risk is expressed in units of mg/m^3. Conversion is done by multiplying the value in mg/kg.d by a value for the body weight of 70 Kg and dividing it by a value for the respiratory rate of 20 m^3/d.

1.4. CHROMIUM (VI)

Parameter	Unit	Value	Source
CAS nr.		7440-47-3	
Type		inorganic	
Molecular weight	g/mol	52	Geometric mean
Solubility	mg/l	-	
Vapour pressure	Pa	0	
Henry coefficient	Pa m³/mol	0	
Kd	dm³/kg	5 [a)]	de Groot et al. (1998)
BCF		[b)]	Ruttens (2005)
Dpe	m²/d	nvt	
Dpvc	m²/d	nvt	
Diffusion coefficient air (Da)	m²/d	calculated	
Diffusion coefficient water (Dw)	m²/d	calculated	
Kp	[cm/h]	$2.00x10^{-3}$	US-EPA (2004b)
FA	-	1	
ABS dermal soil/dust	-	0	dermal contact = mainly local effect
BTF beef	d/kg	$7.46x10^{-3}$	De Raeymaecker et al. (2006)
BTF mutton	d/kg	$7.46x10^{-3}$	= beef
BTF liver	d/kg	$1.80x10^{-3}$	Stevens (1992)
BTF kidney	d/kg	$1.60x10^{-4}$	Stevens (1992)
BTF milk	d/kg	$2.00x10^{-4}$	De Raeymaecker et al. (2006)
BTF soil – egg	d/kg	$3.30x10^{-2}$	= feed - egg
BTF feed - egg	d/kg	$3.30x10^{-2}$	Sheppard et al. (2010)
Carcinogenicity[c)]		1 A Cr(VI)inh D Cr(VI)or	IARC (1990a) US-EPA (1998a) US-EPA (1998a)
Systemic effects threshold			
TDI oral	mg/kg.d	$3x10^{-3}$	US-EPA (1998a)
TCA inhalation[d)]	mg/m³	$1x10^{-2}$	calculated from oral TDI
TDI dermal	mg/kg.d	$7.5x10^{-5}$	oral TDI witht oral absorption factor 0.025
averaging period		child, adolescent, adult	
Local effects threshold			
TCA	mg/m³	$1x10^{-4}$	US-EPA (1998a)
averaging period		lifelong	
Local effects no threshold			
oral slope factor	$(mg/kg.d)^{-1}$		
Unit risk inhalation	$(mg/m^3)^{-1}$	40	WHO (2000)
averaging period		lifelond	
Limit value in air	mg/m³	$2.50x10^{-7}$	WHO (2000)
Limit value in drinking water	mg/m³	50	WHO (WHO, 1996); EC (1998)
Limit value in plants	mg/kg vg	-	
Limit value in meat			
Beef	mg/kg vg	-	
Mutton	mg/kg vg	-	
Liver	mg/kg vg	-	

Parameter	Unit	Value	Source
Kidney	mg/kg vg	-	
Milk	mg/kg vg	-	
Butter	mg/kg vg	-	
Egg	mg/kg vg	-	
Background food adults	mg/kg dag	$5.10x10^{-05}$	Deelstra et al. (1996) (10 % of Cr total)
Background food children	mg/kg.dag	relative with regard to adults cfr. TGD	Cornelis et al. (2013b)
Background potato	mg/kg vg	0.004	MAFF (1999)
Background root crops	mg/kg vg	0.004	MAFF (1999)
Background bulbous plants (onion …)	mg/kg vg	0.004	MAFF (1999)
Background fruit vegetables	mg/kg vg	0.004	MAFF (1999)
Background cabbage	mg/kg vg	0.004	MAFF (1999)
Background leafy vegetables	mg/kg vg	0.002	MAFF (1999)
Background legume	mg/kg vg	0.004	MAFF (1999)
Background beef	mg/kg vg	0.009	MAFF (1999)
Background offal	mg/kg vg	0.008	MAFF (1999)
Background milk	mg/kg vg	0.001	MAFF (1999)
Background butter	mg/kg vg	0.017	MAFF (1999)
Background eggs	mg/kg vg	0.004	MAFF (1999)
Background outdoor air	mg/m^3	$1.30x10^{-6}$	VMM (2004); 25 % of Cr total = Cr(VI)
Background indoor air	mg/m^3	$1.30x10^{-6}$	= outdoor air
Background drinking water	mg/m^3	0	no data

[a] Hexavalent Cr is very mobile. Only at a low pH adsorption of Cr (VI) onto soil occurs (K_d ca. 10-50 l/kg). At a high pH there is hardly any adsorption of Cr(VI) (K_d ca. 1 l/kg; Smolders et al. (2000)). It was decided to adopt a K_d value of 5 l/kg for Cr(VI) which is considered sufficiently conservative for the pH-range 3 – 8.

[b] The choice of BCFs is based on Ruttens (2005). These BCF were derived for total chromium but are used for both Cr(III) and Cr(VI). Calculated and estimated BCF for different crops in the food package are shown in the table below. As salsify, parsnip, paprika, cabbage and maize were not included in the background information to the guidelines on the derivation of soil standards for heavy metals, we defined additional equalisation rules for these crops.

Plant species	BCF or BCF-model	
potatoes		
potatoes	0.019	
root- and tuberous crops	0.003	=carrot
carrots	0.003	
salsify		
Other root crops (e.g. radish)	0.019	= potato
bulbous crops		
bulbous crops (e.g. onion)	0.0004	
leek	0.0004	= onion
fruit vegetables		= tomato
tomato	0.0015	
cucumber	0.0015	= tomato

Plant species	BCF or BCF-model	
Other fruit vegetables (e.g. paprika)		
cabbages	0.019	= potato
cabbage		
cauliflower and broccoli		
Brussels sprouts		
leafy crops		
Lettuce	0.004	
lamb’s lettuce	0.04	= average leafy vegetables from Ruttens (2005)
endive	0.04	= average leafy vegetables from Ruttens (2005)
spinach	0.04	= average leafy vegetables from Ruttens (2005)
Chicory	0.04	= average leafy vegetables from Ruttens (2005)
celery	0.04	= average leafy vegetables from Ruttens (2005)
legume		
beans	0.003	
peas	0.003	= beans
grasses		
grass	0.052	
cereals		
maize	0.052	= grass

c) For the calculation of soil standards chromium (VI) was considered non-carcinogenic via the oral route and carcinogenic via the inhalation route. Therefore both an oral and an inhalation RI were calculated but not summed. As the effect through the oral route is systemic, the S-Risk data sheet also provides an inhalation and dermal toxicological reference value for this endpoint. In addition to the carcinogenic effect by inhalation, there is a toxicological reference value for a local non-carcinogenic effect by inhalation.

d) In the original substance data sheets the reference value for inhalation is expressed in units of mg/kg.d. In contrast the reference value used in S-Risk is expressed in units of mg/m3. Conversion is done by multiplying the value in mg/kg.d by a value for the body weight of 70 Kg and dividing it by a value for the respiratory rate of 20 m^3/d.

1.5. COPPER

Parameter	Unit	Value	Source
CAS nr.		7440-50-8	
Type		inorganic	
Molecular weight	g/mol	63.5	Geometric mean
Solubility	mg/l	-	
Vapour pressure	Pa	0	
Henry coefficient	Pa m³/mol	0	
Kd	dm³/kg	$\log K_d = 1.34 + [0.85 \times \log(0.58 \times \%OM)] + [0.24 \times pH]$ [a)]	Smolders et al. (2000)
BCF		[b)]	Ruttens (2005)
Dpe	m²/d	-	
Dpvc	m²/d	-	
Diffusion coefficient air (Da)	m²/d	calculated	
Diffusion coefficient water (Dw)	m²/d	calculated	
Kp	[cm/h]	1.00×10^{-3}	US-EPA (2004b)
FA	-	1	
ABS dermal soil/dust	-	0	no values for soil and dust; low absorption for copper (European Copper Institute, 2007)
BTF beef	d/kg	[c)]	OVAM (2009d)
BTF mutton	d/kg	7.30×10^{-3}	Sheppard et al. (2010)
BTF liver	d/kg	2.00×10^{-1}	based on Engle et al. (2000)
BTF kidney	d/kg	2.00×10^{-1}	based on Engle et al. (2000)
BTF milk	d/kg	(c)	OVAM (2009d)
BTF soil – egg	d/kg	4.40×10^{-1}	= BTF feed – egg
BTF feed - egg	d/kg	4.40×10^{-1}	Sheppard et al. (2010)
Carcinogenicity		3	IARC (1977, 1987)
Systemic effects threshold			
TDI oral	mg/kg.d	1.6×10^{-1}	WHO (1993, 1998a)
TCA inhalation[d)]	mg/m³	5.6×10^{-1}	calculated from oral TDI
TDI dermal	mg/kg.d	1.3×10^{-1}	from oral TDI with oral absorption factor = 0.8
averaging period		child, adolescent, adult	
Limit value in air	mg/m³	5.60×10^{-1}	calculated from oral TDI
Limit value in drinking water	mg/m³	2000	WHO (1993)
Limit value in plants	mg/kg vg	Grass 6.0 Maize 4.2	EC ("Verordening (EG) nr 1334/2003 van de Commissie van 25 juli 2003 tot wijziging van de toelatingsvoorwaarden voor een aantal toevoegingsmiddelen van de groep sporenelementen in diervoeders," 2003), :adjusted moisture content

Parameter	Unit	Value	Source
Limit value in meat			
Beef	mg/kg vg	-	
Mutton	mg/kg vg	-	
Liver	mg/kg vg	-	
Kidney	mg/kg vg	-	
Milk	mg/kg vg	-	
Butter	mg/kg vg	-	
Egg	mg/kg vg	-	
Background food adults	mg/kg dag	2.00×10^{-2}	Deelstra et al. (1996)
Background food children	mg/kg.dag	relative with regard to adults according to TGD	Cornelis et al. (2013b)
Background potato	mg/kg vg	1	MAFF (1999)
Background root crops	mg/kg vg	1	MAFF (1999)
Background bulbous plants (onion …)	mg/kg vg	1	MAFF (1999)
Background fruit vegetables	mg/kg vg	0.85	MAFF (1999)
Background cabbage	mg/kg vg	0.85	MAFF (1999)
Background leafy vegetables	mg/kg vg	0.76	MAFF (1999)
Background legume	mg/kg vg	0.85	MAFF (1999)
Background beef	mg/kg vg	1.3	MAFF (1999)
Background offal	mg/kg vg	50	MAFF (1999)
Background milk	mg/kg vg	0.05	MAFF (1999)
Background butter	mg/kg vg	0.08	MAFF (1999)
Background eggs	mg/kg vg	0.62	MAFF (1999)
Background outdoor air	mg/m³	1.60×10^{-5}	VMM (2004)
Background indoor air	mg/m³	1.60×10^{-5}	= outdoor air
Background drinking water	mg/m³	2.00×10^{2}	VMM (2006)

a) For the conversion of the K_d value of Cu as a function of pH($CaCl_2$, 0.01 M) and organic carbon (%OC) the following equation is used (R^2 = 0.81; Smolders et al., 2000): log K_d = 1.34 + [0.85 x log(%OC)] + [0.24 x pH]. When %OC is expressed as a function of %OM the following relationship holds:

log K_d = 1.34 + [0.85 x log(0.58 x %OM)] + [0.24 x pH-$CaCl_2$]. A K_d value of 684 l/kg is calculated for a standard soil (pH = 6, %OM = 2 en %OC = 1.16).

b) The choice of BCFs is based on Ruttens (2005). For celery sufficient data existed to allow derivation of a BCF-model[1]. For the other crops data from the international literature are used supplemented with BCF for crops included in the Flemish data set (see table). As salsify, parsnip, paprika, cabbage and maize were not included in the background information to the guidelines on the derivation of soil standards for heavy metals, we defined additional equalisation rules for these crops.

Because the BCF values in literature are derived based on data for non-enriched soils, they possibly overestimate BCF values for enriched soils. Therefore it was decided in close consultation with UHasselt to keep the BCF values as such for a concentration range in soil < 4x Vlarebo background values (background value = 17 mg/kg dm), and to divide the weighted BCF by a metal specific correction factor for soil concentrations > 4x background value.

For copper the reported BCF for root crops (Ruttens, 2005) are divided by a factor 3.14 and for all other vegetables by a factor of 3 for Cu concentrations in soil > 4x background value.

[1] Derived for a pH range of 3.7 to 7.1 and Cu-concentrations in soil of 2 to 155 mg/kg dm.

Plant species	BCF or BCF-model (soil concentration < 4*background value)	
potatoes		
potatoes	0.32	Ruttens (2005)
root- and tuberous crops	0.28	N = carrot
carrots	0.28	Ruttens (2005)
salsify		
Other root crops (e.g. radish)	2.24	= potatoes * 7
bulbous crops		
bulbous crops (e.g. onion)	0.24	Ruttens (2005)
leek	0.24	= onion
fruit vegetables	0.37	N = tomato
tomato	0.37	Ruttens (2005)
cucumber	0.37	= tomato
Other fruit vegetables (e.g. paprika)		
cabbages	0.17	N = cauliflower
cabbage		
cauliflower and broccoli	0.17	Ruttens (2005)
Brussels sprouts	0.17	= cauliflower
leafy crops		
Lettuce	0.35	Ruttens (2005)
lamb's lettuce	0.30	= average above-ground vegetables Ruttens (2005)
endive	0.30	= average above-ground vegetables Ruttens (2005)
spinach	0.30	= average above-ground vegetables Ruttens (2005)
Chicory	0.30	= average above-ground vegetables Ruttens (2005)
selder	log BCFcelery = 0.794 – (0.88 x log Cu) - (0.04 x pH-KCl)	Ruttens (2005)
legume		
beans	0.33	Ruttens (2005)
peas	0.33	= beans
grasses		
grass	0.19	Van Wezel (2003)
cereals		
maize	0.19	N = grass

c) For the derivation of the soil standards and in the excel sheet for heavy metals (OVAM, 2009d) an equation is used to calculate Cu concentrations in meat an milk starting from Cu intake and absorption. In doing so homeostatic processes in the animal were taken into account. These equations were also introduced in S-Risk:

$$C_{meat} = 2.4 * [\text{total intake cow} / (\text{oral absorption cow} * 11)] \wedge 0.0767$$
$$C_{milk} = 0.12 * [\text{total intake cow} / (\text{oral absorption cow} * 11)] \wedge 0.0767$$

Oral absorption equals 0.03.

[d] In the original substance data sheets the reference value for inhalation is expressed in units of mg/kg.d. In contrast the reference value used in S-Risk is expressed in units of mg/m^3. Conversion is done by multiplying the value in mg/kg.d by a value for the body weight of 70 Kg and dividing it by a value for the respiratory rate of 20 m^3/d.

1.6. Inorganic mercury

Parameter	Unit	Value	Source
CAS nr.		7439-97-6	
Type		inorganic	
Molecular weight	g/mol	271.5 ($HgCl_2$)	Geometric mean
Solubility	mg/l	$6.6x10^{4}$	EC (2001)
Vapour pressure	Pa	0 bij 20°C	
Henry coefficient	Pa m³/mol	0 bij 20°C	
Kd	dm³/kg	5706 [a]	Smolders et al. (2000)
BCF		[b]	Ruttens (2005)
Dpe	m²/d	0	
Dpvc	m²/d	0	
Diffusion coefficient air (Da)	m²/d	calculated	
Diffusion coefficient water (Dw)	m²/d	calculated	
Kp	[cm/h]	$1.00x10^{-3}$	US-EPA (2004b)
FA	-	1	
ABS dermal soil/dust	-	$4.00x10^{-1}$	Skowronski et al. (2000)
BTF beef	d/kg	$1.30x10^{-4}$	De Raeymaecker et al. (2006)
BTF mutton	d/kg	$3.00x10^{-2}$	Morgan (1991)
BTF liver	d/kg	$7.80x10^{-3}$	Crout et al. (2004)
BTF kidney	d/kg	$6.40x10^{-2}$	Crout et al. (2004)
BTF milk	d/kg	$1.90x10^{-5}$	De Raeymaecker et al. (2006)
BTF soil – egg	d/kg	0	no data
BTF feed - egg	d/kg	0	no data
Carcinogenicity		**3** **C**	IARC (1993a) US-EPA (1997a)
Systemic effects threshold			
TDI oral	mg/kg.d	$3x10^{-4}$	US-EPA (1997a)
TCA inhalation[c]	mg/m³	$1x10^{-3}$	calculated from oral TDI
TDI dermal	mg/kg.d	$1.2x10^{-4}$	calculated from oral TDI with absorption factor 0.4
averaging period		child, adolescent, adult	
Limit value in air	mg/m³	$1.05x10^{-3}$	calculated from oral TDI
Limit value in drinking water	mg/m³	1	WHO (1993), EC (1998), Vlaamse Regering (2003)
Limit value in plants	mg/kg vg	Grass 0.04 Maize 0.028	based on Belgisch Staatsblad ("Ministerieel Besluit van 12 februari 19991 betreffende de handel en het gebruik van producten die bedoeld zijn voor het voederen van dieren, en wijzigingen," 1999); : adjusted dry matter content; limit values for vegetables no longe rexist in new legislation (EG 1881/2006)
Limit value in meat			

Parameter	Unit	Value	Source
Beef	mg/kg vg	-	
Mutton	mg/kg vg	-	
Liver	mg/kg vg	-	
Kidney	mg/kg vg	-	
Milk	mg/kg vg	-	
Butter	mg/kg vg	-	
Egg	mg/kg vg	-	
Background food adults	mg/kg dag	4.30×10^{-5}	MAFF (1999)
Background food children	mg/kg.dag	relative with regard to adults cfr. TGD	Cornelis et al. (2013b)
Background potato	mg/kg vg	0.001	MAFF (1999)
Background root crops	mg/kg vg	0.001	MAFF (1999)
Background bulbous plants (onion …)	mg/kg vg	0.001	MAFF (1999)
Background fruit vegetables	mg/kg vg	0.0006	MAFF (1999)
Background cabbage	mg/kg vg	0.0006	MAFF (1999)
Background leafy vegetables	mg/kg vg	0.0004	MAFF (1999)
Background legume	mg/kg vg	0.0006	MAFF (1999)
Background beef	mg/kg vg	0.001	MAFF (1999)
Background offal	mg/kg vg	0.005	MAFF (1999)
Background milk	mg/kg vg	0.0004	MAFF (1999)
Background butter	mg/kg vg	0.003	MAFF (1999)
Background eggs	mg/kg vg	0.0013	MAFF (1999)
Background outdoor air	mg/m³	2.24×10^{-6}	VMM (2001)
Background indoor air	mg/m³	2.24×10^{-6}	= outdoor air
Background drinking water	mg/m³	1.00×10^{-1}	VMM (2006)

a) A K_d of 5706 l/kg was derived. It is the median value of 4 observations. No relationship with soil characteristics typical in Flanders could be derived due to a too limited data set.

b) BCF values used in the calculations were derived by Ruttens (2005). BCF values for crops for which no values were available in this report estimations were made based on expert advice (UHasselt) and a limited comparison with available data from research studying metal uptake in food crops (Fytianos, Katsianis, Triantafyllou, and Zachariadis, 2001; Van Wezel, et al., 2003; Versluijs, et al., 2001).
Because the BCF values in literature are derived based on data for non-enriched soils, they possibly overestimate BCF values for enriched soils. Therefore it was decided in close consultation with UHasselt to keep the BCF values as such for a concentration range in soil < 4x Vlarebo background values (background value = 0.55 mg/kg dm), and to divide the weighted BCF by a metal specific correction factor for soil concentrations > 4x background value. For mercury the reported BCF for root crops (Ruttens, 2005) are divided by a factor 3.14 and by a factor of 2.7 for all other vegetables for Hg concentrations in soil > 4x the background value.
For salsify no value exists and therefore a group BCF is defined for root crops which equals that of carrots. For the other fruit vegetables a group BCF value is defined equal to the value of tomatoes. For cabbages a group BCF is defined equal to cabbage,.

Plant species	BCF or BCF-model (soil concentration< 4*background value)	
potatoes		
potatoes	0.25	Ruttens (2005)
root- and tuberous crops	0.29	
carrots	0.29	Ruttens (2005)
schorseneren		
Other **root crops (e.g. radish)**	0.25	= potato
bulbous crops		
bulbous crops (e.g. onion)	0.60	average vegetables Ruttens (2005)
leek	0.60	average vegetables Ruttens (2005)
fruit vegetables	0.072	
tomato	0.072	Ruttens (2005)
cucumber	0.31	Ruttens (2005)
Other fruit vegetables (e.g. paprika)		
cabbages	0.025	
cabbage	0.025	=1/10 potato
cauliflower and broccoli	0.025	= 1/10 potato
Brussels sprouts		
leafy crops		
Lettuce	0.39	Ruttens (2005)
lamb's lettuce	0.60	average vegetables Ruttens (2005)
endive	0.60	average vegetables Ruttens (2005)
spinach	1.62	Ruttens (2005), Fytianos (2001), Versluijs (2001)
Chicory	0.60	average vegetables Ruttens (2005)
celery	0.60	average vegetables Ruttens (2005)
legume		
beans	0.077	Ruttens (2005)
peas	0.077	= beans
grasses		
grass	0.12	Van Wezel (2003)
cereals		
maize	0.12	= grass

[c] In the original substance data sheets the reference value for inhalation is expressed in units of mg/kg.d. In contrast the reference value used in S-Risk is expressed in units of mg/m^3. Conversion is done by multiplying the value in mg/kg.d by a value for the body weight of 70 Kg and dividing it by a value for the respiratory rate of 20 m^3/d.

1.7. METHYL MERCURY

Although methyl mercury is an organic substance it is considered as inorganic in S-Risk because otherwise it would not be possible to make use of bioconcentration factors to calculate plant uptake. This does not influence the results because S-Risk allows to take into account the volatility of inorganic compounds.

Parameter	Unit	Value	Source
CAS nr.		22967-92-6	
Type		inorganic	als invoer in S-Risk
Molecular weight	g/mol	251.1	Geometric mean
Solubility	mg/l	5.50×10^{3} at 25°C	EC (2001)
Vapour pressure	Pa	1.76 at 25°C	EC (2001)
Henry coefficient	Pa m³/mol	0.0803 at 25°C	EC (2001)
log Kow	g/g	0.39794	
log Koc	dm³/kg	-	
Kd	dm³/kg	log K_d = -0.3368 + log % OM	derived from Koc 79.4 l/kg (UK-EA, 2009)
BCF			same values as for inorganic mecury
Dpe	m²/d	0	
Dpvc	m²/d	0	
Diffusion coefficient air (Da)	m²/d	7.44×10^{-1}	UK-EA (2009)
Diffusion coefficient water (Dw)	m²/d	7.44×10^{-5}	UK-EA (2009)
Kp	[cm/h]	1.00×10^{-3}	US-EPA (2004b)
FA	-	1	
ABS dermal soil/dust	-	4.00×10^{-1}	same value as inorganic mercury
BTF beef	d/kg	1.30×10^{-4}	same value as inorganic mercury
BTF mutton	d/kg	3.00×10^{-2}	same value as inorganic mercury
BTF liver	d/kg	7.80×10^{-3}	same value as inorganic mercury
BTF kidney	d/kg	6.40×10^{-2}	same value as inorganic mercury
BTF milk	d/kg	1.90×10^{-5}	same value as inorganic mercury
BTF soil – egg	d/kg	0	same value as inorganic mercury
BTF feed -egg	d/kg	0	same value as inorganic mercury
Carcinogenicity		**2B** **C**	IARC (1993a) US-EPA (1995)
Systemic effects threshold			
TDI oral	mg/kg.d	1×10^{-4}	US-EPA (2001), EC (2001)
TCA inhalation[a)]	mg/m³	3.5×10^{-4}	calculated from oral TDI
TDI dermaal	mg/kg.d	1×10^{-4}	= TDI oral
averaging period		child, adolescent, adult	
Limit value in air	mg/m³	3.5×10^{-4}	calculated from oral TDI[b)]
Limit value in drinking water	mg/m³	1	WHO (1993), EC (1998), Vlaamse Regering (2003)

Parameter	Unit	Value	Source
Limit value in plants	mg/kg vg	Grass 0.04 Mais 0.028	same as inorganic mercury
Limit value in meat			
Beef	mg/kg vg	-	
Mutton	mg/kg vg	-	
Liver	mg/kg vg	-	
Kidney	mg/kg vg	-	
Milk	mg/kg vg	-	
Butter	mg/kg vg	-	
Egg	mg/kg vg	-	
Background food adults	mg/kg dag	$3.79x10^{-5}$	DG Health and Consumer Protection (2004) intake of fish and fish products
Background food children	mg/kg.dag	relative with regard to adults cfr. TGD	Cornelis et al. (2013b)
Background potato	mg/kg vg	0	
Background root crops	mg/kg vg	0	
Background bulbous plants (onion …)	mg/kg vg	0	
Background fruit vegetables	mg/kg vg	0	
Background cabbage	mg/kg vg	0	
Background leafy vegetables	mg/kg vg	0	
Background legume	mg/kg vg	0	
Background beef	mg/kg vg	0	
Background offal	mg/kg vg	0	
Background milk	mg/kg vg	0	
Background butter	mg/kg vg	0	
Background eggs	mg/kg vg	0	
Background outdoor air	mg/m^3	0	
Background indoor air	mg/m^3	0	
Background drinking water	mg/m^3	0	

a) In the original substance data sheets the reference value for inhalation is expressed in units of mg/kg.d. In contrast the reference value used in S-Risk is expressed in units of mg/m^3. Conversion is done by multiplying the value in mg/kg.d by a value for the body weight of 70 Kg and dividing it by a value for the respiratory rate of 20 m^3/d.

b) In the original substance data sheet a wrong limit value in air of 3.5.10 mg/m^3 is provided. The correct value shown here is derived from the oral TDI.

1.8. Elemental mercury

Parameter	Unit	Value	Source
CAS nr.		7439-97-6	
Type		inorganic	
Molecular weight	g/mol	200.6	Geometric mean
Solubility	mg/l	4.94×10^{-2} at 20°C	EC (2001)
Vapour pressure	Pa	0.18 at 20°C	EC (2001)
Henry coefficient	Pa m³/mol	729 at 20°C	EC (2001)
log Kow	g/g	0.623249	
log Koc	dm³/kg	-	
Kd	dm³/kg	5706 [a)]	Smolders et al. (2000)
Log Koa	g/g	-	
BCF			same as inorganic mercury
Dpe	m²/d	0	
Dpvc	m²/d	-	
Diffusion coefficient air (Da)	m²/d	0.548	UK-EA (2009)
Diffusion coefficient water (Dw)	m²/d	0.000173	UK-EA (2009)
Kp	[cm/h]	1×10^{-3}	US-EPA (2004b)
FA	-	1	
ABS dermal soil/dust	-	0	Dermale absorptie beperkt
BTF beef	d/kg	1.3×10^{-4}	same value as inorganic mercury
BTF mutton	d/kg	3.0×10^{-2}	same value as inorganic mercury
BTF liver	d/kg	7.80×10^{-3}	same value as inorganic mercury
BTF kidney	d/kg	6.40×10^{-2}	same value as inorganic mercury
BTF milk	d/kg	1.90×10^{-5}	same value as inorganic mercury
BTF soil – egg	d/kg	0	same value as inorganic mercury
BTF feed - egg	d/kg	0	same value as inorganic mercury
Carcinogenicity		**3** **D**	IARC (1993a) US-EPA (1997b)
Systemic effects threshold			
TDI oral	mg/kg.d	1×10^{-1}	calculated from inhalation value, oral absorption = 0.01 %, inhalation absorption = 69 %
TCA inhalation[b)]	mg/m³	5×10^{-5}	EC (2001)
TDI dermal	mg/kg.d	1×10^{-5}	calculated from inhalation value, inhalation absorption = 69 %
averaging period		child, adolescent, adult	
Limit value in air	mg/m³	5×10^{-5}	EC (2001)
Limit value in drinking water	mg/m³	1	WHO (1993), EC (1998), Vlaamse Regering (2003)
Limit value in plants	mg/kg vg		
Limit value in meat			
Beef	mg/kg vg	0	

Parameter	Unit	Value	Source
Mutton	mg/kg vg	0	
Liver	mg/kg vg	0	
Kidney	mg/kg vg	0	
Milk	mg/kg vg	0	
Butter	mg/kg vg	0	
Egg	mg/kg vg	0	
Background food adults	mg/kg dag	0	
Background food children	mg/kg.dag	0	
Background potato	mg/kg vg	0	
Background root crops	mg/kg vg	0	
Background bulbous plants (onion …)	mg/kg vg	0	
Background fruit vegetables	mg/kg vg	0	
Background cabbage	mg/kg vg	0	
Background leafy vegetables	mg/kg vg	0	
Background legume	mg/kg vg	0	
Background beef	mg/kg vg	0	
Background offal	mg/kg vg	0	
Background milk	mg/kg vg	0	
Background butter	mg/kg vg	0	
Background eggs	mg/kg vg	0	
Background outdoor air	mg/m^3	0	
Background indoor air	mg/m^3	0	
Background drinking water	mg/m^3	0	

[b)] In the original substance data sheets the reference value for inhalation is expressed in units of mg/kg.d. In contrast the reference value used in S-Risk is expressed in units of mg/m^3. Conversion is done by multiplying the value in mg/kg.d by a value for the body weight of 70 Kg and dividing it by a value for the respiratory rate of 20 m^3/d.

1.9. LEAD

Parameter	Unit	Value	Source
CAS nr.		7439-92-1	
Type		anorganisch	
Molecular weight	g/mol	207.2	Geometric mean
Solubility	mg/l	-	
Vapour pressure	Pa	0	
Henry coefficient	Pa m³/mol	0	
Kd	dm³/kg	[a)]	Smolders et al. (2000)
BCF		[b)]	Ruttens (2005)
Dpe	m²/d	0	
Dpvc	m²/d	0	
Diffusion coefficient air (Da)	m²/d	calculated	
Diffusion coefficient water (Dw)	m²/d	calculated	
Kp	[cm/h]	$1.00x10^{-4}$	US-EPA (2004b)
FA	-	1	
ABS dermal soil/dust	-	0	based on data from Boreiko en Battersby (2008)
BTF beef	d/kg	$6.70x10^{-5}$	De Raeymaecker et al. (2006)
BTF mutton	d/kg	$8.91x10^{-2}$	highest value from Van der Veen en Vreman (1986)
BTF liver	d/kg	$3.40x10^{-3}$	Stevens (1992)
BTF kidney	d/kg	$9.00x10^{-3}$	Stevens (1992)
BTF milk	d/kg	$4.90x10^{-5}$	De Raeymaecker et al. (2006)
BTF soil – egg	d/kg	$8.00x10^{-2}$	based on Waegeneers et al. (2009)
BTF feed - egg	d/kg	$1.00x10^{-1}$	based on Waegeneers et al. (2009)
Carcinogenicity		2A (Pb en anorg. Pb-verb.) 3 (Org. Pb-verb.) B2	IARC (2004) US-EPA (1997c)
Systemic effects threshold			
TDI oral	mg/kg.d	$3.6x10^{-3}$	JECFA (1993, 2000), WHO (1993, 1996)
TCA inhalation[c)]	mg/m³	$1.26x10^{-2}$	calculated from oral TDI
TDI dermal	mg/kg.d	$5.4x10^{-4}$	calculated from oral TDI (oral absorption factor 0.15)
averaging period		child, adolescent, adult	
Limit value in air	mg/m³	$5.00x10^{-4}$	WHO (2000)
Limit value in drinking water	mg/m³	10	WHO (1993, 1996)

Parameter	Unit	Value	Source
Limit value in plants	mg/kg vg	Potatoes 0.1 Root crops 0.1 Bulbous plants 0.1 Fruit vegetables 0.1 Cabbage 0.3 Leafy vegetables 0.3 Legume 0.2 Grasss 12 Maize 0.2	EC ("Verordening 1881/2006 van de Commissie van 19 december 2006 tot vaststelling van de maximumgehalten aan bepaalde verontreinigingen in levensmiddelen," 2006) for food (limit value for cereals used for maize) , slightly adjusted list, value for green feed based on Belgisch Staatsblad ("Ministerieel Besluit van 12 februari 19991 betreffende de handel en het gebruik van producten die bedoeld zijn voor het voederen van dieren, en wijzigingen," 1999) only used for grass and not for maize; adjusted dry matter content for feed
Limit value in meat			
Beef	mg/kg vg	0.1	
Mutton	mg/kg vg	0.1	
Liver	mg/kg vg	0.5	EC ("Verordening 1881/2006 van de Commissie van 19 december 2006 tot vaststelling van de maximumgehalten aan bepaalde verontreinigingen in levensmiddelen," 2006)
Kidney	mg/kg vg	0.5	EC ("Verordening 1881/2006 van de Commissie van 19 december 2006 tot vaststelling van de maximumgehalten aan bepaalde verontreinigingen in levensmiddelen," 2006)
Milk	mg/kg vg	0.02	
Butter	mg/kg vg	0.1	EC ("Verordening 1881/2006 van de Commissie van 19 december 2006 tot vaststelling van de maximumgehalten aan bepaalde verontreinigingen in levensmiddelen," 2006)
Egg	mg/kg vg	-	
Background food adults	mg/kg dag	3.70×10^{-4} (31 - < 51 jr;)	Deelstra et al. (1996)
Background food children	mg/kg.dag	1.33×10^{-3} (1 - < 3 jr)	ratio to 3-6 yr taken from EFSA (2010)
		1.13×10^{-3} (3 - < 6 jr)	several studies (OVAM, 2010)
		8.73×10^{-4} (6 - < 10 jr)	verhouding t.o.v. 3-6 jr uit EFSA (2010)
		6.40×10^{-4} (10 - < 15 jr)	verhouding t.o.v. 3-6 jr uit EFSA (2010)
		3.92×10^{-4} (15 - < 21 jr)	verhoudingen t.o.v. 31-51 jr volgens Cornelis et al. (2013b)

Parameter	Unit	Value	Source
		$3.66x10^{-4}$ (21 - < 31 jr)	verhoudingen t.o.v. 31-51 jr volgens Cornelis et al. (2013b)
		$3.66x10^{-4}$ (≥ 51 jr)	verhoudingen t.o.v. 31-51 jr volgens Cornelis et al. (2013b)
Background potato	mg/kg vg	0.003	MAFF (1999)
Background root crops	mg/kg vg	0.003	MAFF (1999)
Background bulbous plants (onion …)	mg/kg vg	0.003	MAFF (1999)
Background fruit vegetables	mg/kg vg	0.015	MAFF (1999)
Background cabbage	mg/kg vg	0.015	MAFF (1999)
Background leafy vegetables	mg/kg vg	0.61	MAFF (1999)
Background legume	mg/kg vg	0.015	MAFF (1999)
Background beef	mg/kg vg	0.006	MAFF (1999)
Background offal	mg/kg vg	0.09	MAFF (1999)
Background milk	mg/kg vg	0.001	MAFF (1999)
Background butter	mg/kg vg	0.005	MAFF (1999)
Background eggs	mg/kg vg	0.003	MAFF (1999)
Background outdoor air	mg/m³	$4.40x10^{-5}$	VMM (2004)
Background indoor air	mg/m³	$4.40x10^{-5}$	=indoor air
Background drinking water	mg/m³	2.5	VMM (2006)

[a] The choice of the partition coefficient K_d is based on the report of Smolders et al. (2000). For the conversion of the K_d-value as a function of soil characteristics following equations were derived::

- pH ≤ 5.5: $\log K_d = 1.76 + (0.4 \times pH)$ $R^2 = 0.92$
- pH > 5.5:
  - $\log(Pb_{tot}) < 3.4 - (0.08 \times pH)$:
    $\log K_d = 1.76 + (0.4 \times pH)$ $R^2 = 0.92$
  - $\log(Pb_{tot}) > 3.4 - (0.08 \times pH)$:
    $\log K_d = -1.64 + (0.48 \times pH) + \log(Pb_{tot})$ theoretical

waarbij de pH bepaald is m.b.v. $CaCl_2$ (0.01 M).

[b] The choice of BCFs is based on Ruttens (2005). For a few crops BCF values are available in this study. For salsify, bulbous crops, fruit vegetables and cabbage no BCFs are available. For salsify a group BCF is adopted equal to the relationship defined for carrots. Also for bulbous crops and fruit vegetables a group BCF was defined. The group BCF for cabbage equals the value for Brussels sprouts. The BCF for grass was derived from the average value of all values reported in (2001).

Plant species	BCF or BCF-model	
potatoes		
potatoes	Log BCF = -1.09 – 0.84 log Pb_{soil}	Ruttens (2005)
root- and tuberous crops		= carrots
carrots	Log BCF = 0.36 – 0.23 pH – 0.61 log Pb_{soil}	Ruttens (2005)
salsify		
Other root crops (e.g. radish)	0.012	= median value potato*4 for standard soil
bulbous crops	0.00475	= value leafy vegetables/2 for standard soil
bulbous crops (e.g. onion)		

Plant species	BCF or BCF-model	
prei		
fruit vegetables	0.003	= median value potato for standard soil
tomato		
cucumber		
Other fruit vegetables (e.g. paprika)		
cabbages	0.00317	
cabbage		
cauliflower and broccoli	0.003	median value potato for standard soil
Brussels sprouts	0.0032	=value leafy vegetables / 3
leafy crops		
Lettuce	$\text{Log } Pb_{plant} = -0.9 + 0.68 \text{ log } Pb_{soil}$	Ruttens (2005)
lamb's lettuce	0.0095	= value leafy vegetables
endive	0.0095	= value leafy vegetables
spinach	0.0095	= value leafy vegetables
Chicory	0.0032	= value leafy vegetables / 3
celery	$\text{Log } Pb_{plant} = -1.23 + 0.84 \text{ log } Pb_{soil}$	Ruttens (2005)
legume		
beans	0.006	= median value potato * 2 for standard soil
peas	0.003	= median value potato for standard soil
grasses		
grass	0.04439	= average Versluijs en Otte (2001)
cereals		
maize	$\text{log } Pb_{plant} = -1.63 + 1.16 \text{ log } Pb_{soil}$	Ruttens (2005)

[c] In the original substance data sheets the reference value for inhalation is expressed in units of mg/kg.d. In contrast the reference value used in S-Risk is expressed in units of mg/m^3. Conversion is done by multiplying the value in mg/kg.d by a value for the body weight of 70 Kg and dividing it by a value for the respiratory rate of 20 m^3/d.

1.10. NICKEL

Parameter	Unit	Value	Source
CAS nr.		8049-31-8	
Type		inorganic	
Molecular weight	g/mol	58.7	Geometric mean
Solubility	mg/l	-	
Vapour pressure	Pa	0	
Henry coefficient	Pa m³/mol	0	
Kd	dm³/kg	[a)]	Smolders et al. (2000)
BCF		[b)]	Ruttens (2005)
Dpe	m²/d	0	
Dpvc	m²/d	0	
Diffusion coefficient air (Da)	m²/d	calculated	
Diffusion coefficient water (Dw)	m²/d	calculated	
Kp	[cm/h]	$2.00x10^{-4}$	US-EPA (2004b)
FA	-	1	
ABS dermal soil/dust	-	0	low dermal absorption from soil is assumed
BTF beef	d/kg	$6.80x10^{-4}$	De Raeymaecker et al. (2006)
BTF mutton	d/kg	$6.80x10^{-4}$	= beef
BTF liver	d/kg	$3.00x10^{-4}$	Stevens (1992)
BTF kidney	d/kg	$8.10x10^{-4}$	Stevens (1992)
BTF milk	d/kg	$2.70x10^{-5}$	De Raeymaecker et al. (2006)
BTF soil – egg	d/kg	$2.70x10^{-1}$	= BTF feed-egg
BTF feed - egg	d/kg	$2.70x10^{-1}$	Sheppard et al. (2010)
Carcinogenicity		1 (Ni-compounds)	IARC (1990b, 1999)
		2B (Ni(0))	IARC (1990b, 1999)
		A (Ni- refinary dust and Ni-subsulphide)	US-EPA (1997e, 1997f)
		B2 (Ni-carbonyl)	US-EPA (1997d)
Systemic effects threshold			
TDI oral	mg/kg.d	$2x10^{-2}$	US-EPA (1998d)
TCA inhalation[c)]	mg/m³	$2.0x10^{-5}$	EC (2004)
TDI dermal	mg/kg.d	$1x10^{-4}$	calculated from oral TDI met oral absorption factor 0.05
averaging period		child, adolescent, adult	
Local effects non-threshold			[d)]
Unit risk[e)] inhalation	$(mg/m^3)^{-1}$	$3.8x10^{-1}$	WHO (2000)
averaging period		lifelong	
Limit value in air	mg/m³	$2.00x10^{-5}$	EC (2004)
Limit value in drinking water	mg/m³	20	WHO (1998b)
Limit value in plants	mg/kg vg		
Limit value in meat			
Beef	mg/kg vg	-	
Mutton	mg/kg vg	-	
Liver	mg/kg vg	-	
Kidney	mg/kg vg	-	
Milk	mg/kg vg	-	

Parameter	Unit	Value	Source
Butter	mg/kg vg	-	
Egg	mg/kg vg	-	
Background food adults	mg/kg dag	1.90×10^{-3}	MAFF (1999)
Background food children	mg/kg.dag	relative with regard to adults cfr. TGD	Cornelis et al. (2013b)
Background potato	mg/kg vg	0.062	MAFF (1999)
Background root crops	mg/kg vg	0.062	MAFF (1999)
Background bulbous plants (onion …)	mg/kg vg	0.062	MAFF (1999)
Background fruit vegetables	mg/kg vg	0.078	MAFF (1999)
Background cabbage	mg/kg vg	0.078	MAFF (1999)
Background leafy vegetables	mg/kg vg	0.088	MAFF (1999)
Background legume	mg/kg vg	0.078	MAFF (1999)
Background beef	mg/kg vg	0.12	MAFF (1999)
Background offal	mg/kg vg	0.0016	MAFF (1999)
Background milk	mg/kg vg	0.005	MAFF (1999)
Background butter	mg/kg vg	0.04	MAFF (1999)
Background eggs	mg/kg vg	0.017	MAFF (1999)
Background outdoor air	mg/m³	6.20×10^{-6}	VMM (2004)
Background indoor air	mg/m³	6.20×10^{-6}	= outdoor air
Background drinking water	mg/m³	2.5	VMM, 2006

[a] To convert the K_d value for Ni as a function of pH($CaCl_2$, 0.01 M) followoing equation is used (R^2 = 0.71): log K_d = 1.31 + (0.25 x pH). For a standard soil a K_d value of 646 l/kg is calculated.

[b] The BCFs for Ni are based on expert advice (UHasselt/VITO) and a limited comparison with available data from research studying metal uptake in food crops.
Because the BCF values in literature are derived based on data for non-enriched soils, they possibly overestimate BCF values for enriched soils. Therefore it was decided in close consultation with UHasselt to keep the BCF values as such for a concentration range in soil < 4x Vlarebo background values (background value = 9 mg/kg dm), and to divide the weighted BCF by a metal specific correction factor for soil concentrations > 4x background value. The way the weighted BCF and correction factors are determined is explained in a separate chapter included in Ruttens (2005). For nickel the reported BCF for root crops (Ruttens, 2005) are divided by a factor 3.14 and by a factor of 1.7 for all other vegetables for Ni concentrations in soil > 4x background value.
Because no data exist for salsify a group BCF equal to the value for carrots was adopted. Fruit crops different from tomato and cucumber were assigned a group BCF equal to this of tomatoes. Also for cabbages a group BCF was defined.

Plant species	BCF or BCF-model (soil concentration < 4*background value)	
potatoes		
potatoes	0.051	Ruttens (2005)
root- and tuberous crops	0.026	= value carrots
carrots	0.026	Ruttens (2005)
salsify		
Other root crops (e.g. radish)	0.051	= value potatoes
bulbous crops		
bulbous crops (e.g. onion)	0.038	Ruttens (2005)

Plant species	BCF or BCF-model (soil concentration < 4*background value)	
leek	0.038	= uien
fruit vegetables	0.025	N = tomato
tomato	0.025	Ruttens (2005)
cucumber	0.105	Ruttens (2005)
Other fruit vegetables (e.g. paprika)		
cabbages	0.041	N = cauliflower
cabbage		
cauliflower and broccoli	0.041	Ruttens (2005)
Brussels sprouts		
leafy crops		
Lettuce	0.081	Ruttens (2005)
lamb's lettuce	0.081	= Lettuce
endive	0.081	= Lettuce
spinach	0.081	= Lettuce
Chicory	0.081	= Lettuce
celery	0.081	= Lettuce
legume		
beans	0.14	Ruttens (2005)
peas	0.14	=beans
grasses		
grass	0.098	Ruttens (2005)
cereals		
maize	0.098	N = grass

c) In the original substance data sheets the reference value for inhalation is expressed in units of mg/kg.d. In contrast the reference value used in S-Risk is expressed in units of mg/m^3. Conversion is done by multiplying the value in mg/kg.d by a value for the body weight of 70 Kg and dividing it by a value for the respiratory rate of 20 m^3/d. d) For the derivation of the soil standards Ni was concidered non-carcinogenic. In S-Risk also local carcinogenic effects via inhalation are considered. This should not have an impact on the risk assessment as non-carcinogenic effects are critical for Ni. e) In the original substance data sheets the screening values for non-threshold carcinogenic effects is given for a lifelong dose and a $1/10^5$ extra cancer incidence. S-Risk uses slope factors and unit risks. Conversion is as follows: Slope factor $((mg/kg.d)^{-1}) = 1x10^{-5}/(\text{dose for } 1x10^{-5} (mg/kg.d))$. For inhalation a prededing conversion from mg/kg.d to mg/m^3 should be done by multiplication by 70 kg (body weight) and division by 20 m^3/d (respiratory volume).

1.11. Zinc

Parameter	Unit	Value	Source
CAS nr.		7440-66-6	
Type		inorganic	
Molecular weight	g/mol	65.4	Geometric mean
Solubility	mg/l	-	
Vapour pressure	Pa	0	
Henry coefficient	Pa m³/mol	0	
Kd	dm³/kg	[a)]	Smolders et al. (2000)
BCF		[b)]	Ruttens (2005)
Dpe	m²/d	0	
Dpvc	m²/d	0	
Diffusion coefficient air (Da)	m²/d	calculated	
Diffusion coefficient water (Dw)	m²/d	calculated	
Kp	[cm/h]	6.00x10^{-4}	US-EPA (2004b)
FA	-	1	
ABS dermal soil/dust	-	0	Bierkens et al. (2006)
BTF beef	d/kg	[c)]	
BTF mutton	d/kg	1.20x10^{-1}	Sheppard et al. (2010)
BTF liver	d/kg	1.20x10^{-1}	Sheppard et al. (2010)
BTF kidney	d/kg	1.20x10^{-1}	Sheppard et al. (2010)
BTF milk	d/kg	(c)	
BTF soil – egg	d/kg	1.10	= BTF feed-egg
BTF feed - egg	d/kg	1.10	Sheppard et al. (2010)
Carcinogenicity		D	US-EPA (1998c)
Systemic effects threshold			
TDI oral	mg/kg.d	5x10^{-1}	Baars et al. (2001), EC (1993)
TCA inhalation[d)]	mg/m³	1.75	calculated from oral TDI
TDI dermal	mg/kg.d	1.5x10^{-1}	calculated from oral TDI with oral absorption factor 0.3
averaging period		child, adolescent, adult	
Limit value in air	mg/m³	1.75	= TCA inhalation
Limit value in drinking water	mg/m³	5000	B. Vl. Reg. (1989)
Limit value in plants	mg/kg vg	Grass 60 Maize 42	afgeleid uit lijst in uitvoering van EC ("Verordening (EG) Nr 1831/2003 van het Europees Parlement en de Raad van 22 september 2003 betreffende toevoegingsmiddelen voor diervoeding," 2003)
Limit value in meat			
Beef	mg/kg vg	-	
Mutton	mg/kg vg	-	
Liver	mg/kg vg	-	
Kidney	mg/kg vg	-	
Milk	mg/kg vg	-	
Butter	mg/kg vg	-	
Egg	mg/kg vg	-	

Parameter	Unit	Value	Source
Background food adults	mg/kg dag	1.57×10^{-1}	Deelstra et al. (1996) en Hendrix et al. (1998)
Background food children	mg/kg.dag	relative with regard to adultscfr. TGD	Cornelis et al. (2013b)
Background potato	mg/kg vg	3.3	MAFF (1999)
Background root crops	mg/kg vg	3.3	MAFF (1999)
Background bulbous plants (onion …)	mg/kg vg	3.3	MAFF (1999)
Background fruit vegetables	mg/kg vg	2.4	MAFF (1999)
Background cabbage	mg/kg vg	2.4	MAFF (1999)
Background leafy vegetables	mg/kg vg	3.9	MAFF (1999)
Background legume	mg/kg vg	2.4	MAFF (1999)
Background beef	mg/kg vg	52	MAFF (1999)
Background offal	mg/kg vg	52	MAFF (1999)
Background milk	mg/kg vg	3.9	MAFF (1999)
Background butter	mg/kg vg	0.5	MAFF (1999)
Background eggs	mg/kg vg	13	MAFF (1999)
Background outdoor air	mg/m³	4.87×10^{-5}	VMM (2004)
Background indoor air	mg/m³	4.87×10^{-5}	= outdoor air
Background drinking water	mg/m³	2.17×10^{2}	VMM (2006)

a) For the conversion of the K_d value for Zn as a function of pH($CaCl_2$, 0.01 M) following equation is used ($R^2 = 0.75$): $\log K_d = -1.09 + (0.61 \times pH)$. At pH = 6 a K_d value of 372 l/kg is obtained.

b) The choice of appropriate BCF values is documented in Ruttens (2005). The most important aspects are summarised below.
The BCF values were to the extent possible derived from Flemish data and are subdivided in three sub-categories according to the enrichment of Zn in the soil :

- Zn-concentration in soil <60 mg/kg ds (background value):
  - Potatoes: 0.58;
  - Other root crops: 0.85;
  - Celery: regression model (see below)
  - Spinach:4.29
  - Other leafy vegetables:3.55
  - Other above-ground vegetables: 0.5
- Zn-concentration in soil 60- 360 mg/kg ds:
  - Potato: 0.11
  - Other root crops: 0.61
  - Celery: regressionmodel (see below)
  - Spinach:1.5
  - Other leafy vegetables:0.82
  - Other above-ground vegetables: 0.32
- Zn-concentration in soil >360 mg/kg ds
  - Potato: 0.055
  - carrot:0.14
  - radish:0.46
  - Other root crops: 0.30
  - Celery: regressionmodel (see below)
  - Spinach: 0.77
  - Lettuce:0.38
  - Other leafy vegetables:0.41

- Beans: 0.13
- Cucumber: 0.18
- Other above-ground vegetables: 0.16

For celery sufficient data were available in Ruttens (2005) in order to derive a regression model for the entire concentration range

$$\log BCF_{celery} = 2.34 - (0.48 \times \log Zn) - (0.22 \times pH)$$

The BCF value for grass was obtained from Van Wezel et al. (2003).

For certain vegetables no BCF values were available from the calculation of the soil standards. For salsify a group BCF for root crops was used. For fruit crops a group BCF is used equal to tomatoes. Bulbous crops and cabbage are each evaluated as a group. The BCF for maize was set equal tot that of grass.

c) For the derivation of the soil standards and in the spreadsheet for heavy metals (OVAM, 2009d) an equation is used to calculate Zn concentrations in meat an milk starting from Zn intake and absorption. In doing so homeostatic processes in the animal were taken into account. These equations were also introduced in S-Risk:

$$C_{meat} = 21.28 * [\text{total intake cow} / (\text{oral absorption cow} * 11)] \wedge 0.1621$$
$$C_{milk} = 2.66 * [\text{total intake cow} / (\text{oral absorption cow} * 11)] \wedge 0.1621$$

Oral absorption was set equal to 0.2.

d) In the original substance data sheets the reference value for inhalation is expressed in units of mg/kg.d. In contrast the reference value used in S-Risk is expressed in units of mg/m^3. Conversion is done by multiplying the value in mg/kg.d by a value for the body weight of 70 Kg and dividing it by a value for the respiratory rate of 20 m^3/d.

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