September 2021

Development of Screening Levels in soil and groundwater in Wallonia

Technical document for the selection of appropriate physical-chemical properties and toxicity values of chemical compounds

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PURPOSE OF SCREENING LEVELS IN SOIL AND GROUNDWATER

Soil legislation in Wallonia was enforced through the first Soil Decree passed in December 2008 and further renewed in March 2018. During the soil and groundwater investigations, several chemical compounds of interest and linked to the past/current industrial activities are measured. The Soil Decree provides trigger values for 50 usual pollutants (metals, BTEX, PAH, TPH and chlorinated solvents). When a chemical is targeted and quantified but not considered as a usual pollutant, the Soil Decree requests two public institutes specialized in the environmental field, ISSeP[1] and SPAQuE[2], to be in charge of developing soil and groundwater screening values for these chemicals.

In the same way as the "Regional Screening Levels" provided by US-EPA for 800 chemicals[3], the screening levels calculated here are chemical-specific concentrations for individual contaminants in soil and groundwater that warrant further investigation or site clean-up. This guidance sets forth a recommended, but not mandatory, approach based upon currently available information. **It should be emphasized that these screening levels are not clean-up standards**.

The aim of this technical document is to keep the traceability (principle of transparency) about the calculated values and to allow other stakeholders in Wallonia to calculate the screening values by their own, following this document endorsed by the Walloon Administration of Environment.

For this, ISSeP and SPAQuE have developed a procedure to search and select the physical and chemical properties of the chemicals, as well as toxicity data, needed to calculate the screening levels. These parameters are used to identify the potential fate of the chemicals in the environment. There are many sources for physical-chemical parameter values, but unfortunately the values listed in various sources can sometimes differ. This procedure specifies the reference sources and the hierarchy for the selection of the appropriate values.

The screening levels are based on the risk assessment methodology followed in Wallonia and described in details in the "Walloon Guide for Good Practices"[4]. The tables provide screening levels corresponding to either a 10^{-5} risk level for non-threshold effect

[1] http://www.issep.eu/ for English version
[2] http://www.english.spaque.be/01215/fr/Home for English version
[3] https://www.epa.gov/risk/regional-screening-levels-rsls-users-guide
[4] http://dps.environnement.wallonie.be/home/sols/sols-pollues/code-wallon-de-bonnes-pratiques--cwbp-.html (only in French version)

substances, i.e. substances exhibiting adverse effects unless the exposure level is zero or a Hazard Quotient of 1 for substances acting with threshold. The lowest value is retained for a both non–threshold and threshold chemical.

These parameters allow to calculate 2 **soil** screening levels:

- a human health screening level, calculated with S-RISK WAL® tool (**VITO, 2017**[5]), called **VL_H** (VL stands for *Valeur Limite*; Limit Value in French), following the risk assessment methodology defined by the National Research Council, in USA (**NRC, 1983**[6]), in the reverse mode, using conservative assumptions. The screening levels are calculated for 5 land uses (natural, agricultural, residential, park/commercial and industrial) ;
- a groundwater leaching screening level, calculated by equations adjusted on Connor model (**Connor, 1997**[7]), called **VL_N**, to evaluate leaching and dispersion of soil pollutant into groundwater.

These parameters allow to calculate 2 **groundwater** screening levels:

- a human health screening level, similar to drinking water criteria (for tap water), called **VL_nappe**;
- a human health screening level, taking into account the volatilization of a volatile chemical in groundwater through the soil layer, called **VL_nappe_volatilisation**.

Some steps, specific to S-RISK WAL® tool, are indicated *in italic*.

All the selected physical-chemical parameters, the toxicity values and the screening levels are collected in an Excel file, available on the Walloon Administration for Environment website: https://sol.environnement.wallonie.be/home/documents/le-coin-des-specialistes-experts-laboratoires/polluants-non-normes-pnn.html

STEP 1 : The chemical identity

For each chemical, the first step consists of searching the corresponding CAS Registry number (Chemical Abstracts Service) – which is the key number - and synonyms as well, to avoid confusion.

List of reference sources:

[1] TOXNET – ChemIDplus (web) = the most complete database (400 000 substances) (http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp).

But also:

[2] TOXNET - HSDB - Hazardous Substances Data Bank (web) (https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm);

[3] Lide D. (2009-2010) - « CRC Handbook of Chemistry and Physics » 90th Edition;

[4] Mackay D. *et al.* (2006) - « Handbook of Physical-Chemical Properties and Environmental Fate for organic Chemicals » Vol I - IV - Second Edition;

[5] VITO (2017), Cornelis C. *et al*. S-RISK version for the Walloon region : Technical guidance document, February 2017
[6] NRC (1983), Risk assessment in the federal government. Managing the process. Washington. D.C, National Academy of Science, 191 p.
[7] Connor J. *et al.* (1997), Soil attenuation model for derivation of risk-based soil remediation standards, Groundwater Services Inc, July 1997

[5] Verschueren K. (1996) - « Handbook of environmental data on organic chemicals »- latest report (2008)

If no CAS number existing → STOP
If CAS number existing → steps 2 and 3

STEP 2 : The carcinogenic classification

A chemical may be a carcinogen, a mutagen or a teratogen. Several institutes (IARC,[8] NTP[9], European Union, US EPA[10]) are in charge of their evaluation then identify some of them as carcinogenic, probably carcinogenic, or possibly carcinogenic to humans.

The whole protocol developed by ISSeP (« Développement d'une Procédure pour la Sélection des Valeurs Toxicologiques de Référence et la Prise en Compte du Caractère Cancérogène d'un Polluant », ISSeP, Août 2016, Rapport n°01881*)* will not be detailed, only the key information is summarized here.

For each chemical, the carcinogenic classification done by the following institutes is collected:

- IARC[11];
- NTP[12];
- European Union;
- US EPA[13].

STEP 3 : The selection of the Toxicity Reference Values (TRV)

The Toxicity Reference Value (TRV) is derived from the dose-response assessment which establishes a relationship between the exposure to a substance and a human adverse effect.

For a chemical, until 4 TRV may be available: separately for threshold effects and non-threshold effects, for respiratory and oral routes. Most often, the TRV for oral route replaces the missing TRV dedicated to the dermal route (see the units in Table 1).

[8] International Agency for Research on Cancer
[9] National Toxicology Program
[10] United States Environmental Protection Agency
[11] International Agency for Research on Cancer
[12] National Toxicology Program
[13] United States Environmental Protection Agency

Table 1: Toxicity reference values and units

Type of effect / Route	Inhalation	Oral	Dermal
Threshold effect = non carcinogenic effect and carcinogenic non genotoxic effect	mg/m^3	mg/kg·j	mg/kg·j
Non-threshold effect = carcinogenic and genotoxic effect	$(mg/m^3)^{-1}$	$(mg/kg \cdot j)^{-1}$	$(mg/kg \cdot j)^{-1}$

The whole protocol developed by ISSeP (« Développement d'une Procédure pour la Sélection des Valeurs Toxicologiques de Référence et la Prise en Compte du Caractère Cancérogène d'un Polluant », ISSeP, Août 2016, Rapport n°01881*)* will not be detailed, only the key information is summarized here.

The collation and the selection of the relevant TRV is done in three steps. Only TRV elaborated for **a chronic exposure** are considered (exposure duration > 1 year).

In the first step, the TRV are collected in the following international databases (Level 1):
- WHO,
- JECFA,
- EFSA,
- US-EPA (IRIS),
- ATSDR.

In the second step, the TRV are collected in the databases from national institutes (Level 2):
- US-EPA (PPRTV),
- OEHHA (California),
- ANSES (France),
- Health Canada (Canada),
- RIVM (The Netherlands).

If several values are available for one route and for an effect, only the hierarchy Level 1 / 2 and the date of publication (last revised) will be taken into account for the selection of the **relevant** value:
- Priority for recent TRV (< 10 years) AND the most protective value in the databases of Level 1;
- If no recent TRV is available in the databases of Level 1, recent TRV of Level 2 or older TRV (> 10 years) coming from the Level 1 are considered. The final choice is often leaded by the most protective value of the set.

If no TRV is available in the usual databases, the third step consists of collecting data in other databases (occupational exposure for example) for deriving an "Indicative Toxicity Value" (and not a TRV, due to uncertainties). This step has to be done by an Expert in toxicology field.

STEP 4 : Selection of the physical-chemical properties

1. List of properties

The following physical and chemical properties are needed for calculating the soil screening values.

Table 2: Physical and chemical properties

Properties	Symbols	Units
Molecular formula	-	-
SMILES formula	-	-
Molecular weight	M	g/mol
Vapour pressure **at 10 °C**	P	Pa
Henry's Law Constant **at 10°C**	H	Pa.m³/mol
Solubility in water **at 10°C**	S	mg/L
Soil-water partition coefficient for inorganics	Kd	L/kg
Octanol-water partition coefficient	Kow	-
Organic carbon-water partition coefficient	Koc	L/kg
Acid dissociation constant in water	pKa	-
Acid or base ? (if pKa available)	-	-
Permeation coefficient through polyethylene (PE) drinking-water service pipe	Dpe	m²/j
Bioconcentration Factor in plants	BCF	For inorganics : $(mg/kg_{dw\ plant})/(mg/kg_{dw\ soil})$ *For organics in S-RISK WAL®: $(mg/kg_{dw})/(mg/m^3)$*
Biotransfer factor to beef meat, sheep meat, kidney, milk and egg	BTF	$(mg/kg_{fw})/(mg/j)$
Dermal permeability coefficient of compound in water	Kp	cm/h
Dermal absorption factor from soil	ABS_dermal, soil/dust	-
Fraction of absorbed water	FA	-

In S-RISK WAL® model, some parameters as Da (diffusion coefficient in air), Dw (diffusion coefficient in water) and Koa (octanol-air partition coefficient) are calculated by the model and don't need to be selected. The parameter D_{pvc} (the permeation coefficient for PVC water pipes) has not to be filled in because polyethylene water pipes are considered by default in the standard land uses.

2. CONSULTED DATABASES

The physical and chemical properties, showing the chemical fate in soil and water, are documented in Handbooks or databases available on the web. The properties are collected in the following list of reference sources:

List 1 - priority

[1] Pubchem (https://pubchem.ncbi.nlm.nih.gov/)

[2] Mackay D. *et al.* (2006) - « Handbook of Physical-Chemical Properties and Environmental Fate for organic Chemicals » Vol I - IV - Second Edition;

[3] Syracuse Research Center (SRC) (http://esc.syrres.com/fatepointer/search.asp) – PHYSPROP Database.[14]

The previous databases have been firstly chosen because they are a recent data compilation coming from many and validated reference sources (Mackay *et al.*, 2006) or because they are the recommended sources by other regions/countries:

- US-EPA recommends SRC-PHYSPROP;
- OVAM (Flemish Institute, Belgium) recommends Mackay et *al*. (2006) and SRC-Physprop;
- INERIS (France) recommends Mackay *et al.* (2006).

If no value is available in these databases for a property, the databases of the List 2 are used (no complete list):

List 2

[1] IUPAC (http://sitem.herts.ac.uk/aeru/iupac/);

[2] ATDSR - Agency for Toxic Substances and Disease Registry (http://www.atsdr.cdc.gov/toxprofiles/index.asp);

[3] Lide D. (2009-2010) - « CRC Handbook of Chemistry and Physics » 90th Edition;

[4] Lijzen et *al.* (February 2001). « Technical evaluation of the Intervention values for soil/sediment and groundwater » RIVM report 711701 023 (link);

[5] Sander R. (2015) Compilation of Henry's law constants (version 4.0) for water as solvent. Atmos. Chem. Phys,15, 4399-4981. Useful for H data (link);

[6] SPAQuE (2015). Projet POLLUSOL 2 (2009-2015) – rapport de synthèse – version finale du 10 février 2015, useful for BCF of Al, Ba, Be, Co, Mo, Sb, Se, Sn and Mn – *in French* (link);

[7] Cullen A. and *al.* (1996). Influence of harbor contamination on the level and composition of polychlorinated biphenyls in produce in Greater New Bedford, Massachusetts, Environmental Science and Technology vol.30 n°5, especially for PCB's BCF in plants;

[8] US EPA - Regional Screening Levels (RSLs) - User's Guide – Generic Tables – Chemical parameters (https://www.epa.gov/risk/regional-screening-levels-rsls-generic-tables-november-2017), useful for Kd;

[9] RAIS[15] (link)

[10] INERIS - Fiches environnementales et toxicologiques *in French* (link) ;

[11] INRS - Fiches toxicologiques *in French* (http://www.inrs.fr/publications/bdd/fichetox.html) ;

[12] US EPA, EPI software « EPIWEB » (https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

[14] SRC PHYSPROP website is currently not available. Some physico-chemical properties from SRC-PHYSPROP are taken up again in HSDB.

[15] RAIS, Risk Assessment Information System

[13] Verschueren K. (1996 ; 2008) - « Handbook of environmental data on organic chemicals » (This database was downgrade to list 2 in december 2020).

3. SELECTION OF PROPERTIES

General recommendations

- Experimental (measured) values are preferred to calculated, estimated or extrapolated values ;

- The properties values are selected in databases following an order of preference (1, 2, 3, 4) indicated in the following table. If no value is available, look the other databases and select the most protective value or the most relevant value. If several values are available in a single database at the same temperature, calculate the geometric mean of the consistent values (5 values minimum). Check the consistency with another database from List 1 or List 2, at least.

- When available, values obtained at 10 °C (±2.5°C) are preferred to others, which is the annual mean soil temperature in a temperate oceanic climate. The selection of Henry's Law constant H (Pa·m³/mol), vapour pressure P (Pa) and solubility in water S (mg/L) will be ideally chosen at soil or ambient temperature (vapour pressure is the most sensitive property with temperature). If no H value is available in List 1 and List 2, the S and P properties will be selected at the same temperature in order to obtain a consistent H, often calculated by the model (*as S-RISK WAL® for example).*

- If several values for a property seem to be inconsistent, another value may be selected, with appropriate justifications.

Recommendations for each property

Parameters in « Chemical » (S-RISK WAL®)	**Recommendations**
Molecular weight **M**	First choice 1: Mackay *et al.* (2006) 2: other databases of List 1 3: databases of List 2
Henry's Law constant **H**	For Organic chemicals : First choice 1: Mackay *et al.* (2006) 2: other databases of List 1 3: databases of List 2 4: H will be calculated on the basis of S, P, and M values at the same temperature. If several values are available at different temperatures, the selection will be done as follows, in the order of priority : a. If available, select the experimental value at 10°C (±2.5°C) b. If several experimental values at 10 °C (±2.5°C) are available, select the higher value (the most conservative) or the most relevant one c. If available, select the experimental value at 20°C (±5°C) in

	the lowest part of the temperature range d. if available and consistent (5 values minimum at the same temperature, the lowest possible), calculate the geometric mean of the experimental values at 20°C (±5°C) e. If no experimental value is available in List 1, calculate the geometric mean of extrapolated values/ obtained by equations, at the 10 °C temperature (5 values minimum) in Mackay et *al.* The equations of H containing K_{AW}[16] mustn't be taken into account f. Idem than e) but at 20°C (±5°C) Anyway, the use of equations has to be avoided and if needed, the calculated value must be compared to other values to check the consistency **Caution: the values given at non usual pressure or temperature (example: « supercooled liquids ») cannot be selected.** For inorganic chemicals : *Set the value at « 0 » (aberrant value) and temperature at "20°C".*
Solubility in water **S**	For organic chemicals : - If H value has been already selected in the usual databases, select the value of PUBCHEM (HSDB priority) for **S**. - If H value is not available in the usual databases, select **S** value following the methodology for **H.** For inorganic chemicals : *Set the value at de « 1.0E47 » (aberrant value).*
Vapor Pressure **P**	For organic chemicals : - If H value has been already selected in the usual databases, select the value of PUBCHEM (HSDB priority) for **P**. - If H value is not available in the usual databases, select **P** value following the methodology for **H.** Conversion factor: 1 atm = 760 mmHg = 101325 Pa. For inorganic chemicals : *Set the value at « 0 » (aberrant value) and temperature at "20°C".*
Log octanol/water partition coefficient **log Kow**	Select the value of **log Kow** in PUBCHEM (HSDB priority).
Log organic carbon/water partition	First choice 1: Mackay *et al.* (2006) 2: other databases of List 1 3: databases of List 2 4: calculation with MCI method in EPIWEB (US-EPA tool) (https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface). In Mackay et *al*. (2006), if more than 5 values are available, calculate the geometric mean of the experimental values, ideally at

[16] Air-water partition coefficient is linked to Henry'Law Constant by the relationship K_{AW} = H/R.T

coefficient **log Koc**	the same temperature. In Mackay et *al*. (2006), if less than 5 values are available, select the lowest one (the most conservative). Caution : when calculating the geometric mean, do not select : - Values coming from mineral or organic matter which is not soil (for example: sediment, aquifer material, humic acid soil, sewage sludge, zeolithe, clay minerals, etc.); - Values elaborated from experiments where soils are mixed with chemicals as $CaCl_2$, EDTA, etc. - Values obtained at very high or very low pH (for example: speciation study). If data are a mean value and its range (min. and max.), select only the mean value. If data consists of a range (min. and max.), select these both values separately for the calculation. *Caution : avoiding Koc calculation by S-RISK WAL®*
Acid dissociation constant in water **pKa**	First choice 1: SRC-PHYSPROP 2: other databases of List 1 3: databases of List 2 Caution : pKa must be elaborated in aqueous environment
Acid or base	For pesticides, select the value from IUPAC database For other chemicals, select the value from ATSDR Caution: Only pKa between 2 and 12 must be taken into account. Otherwise (pKa <2 or pKa >12), the chemical is not protonated/ deprotonated in water (no acid/basic property in water) or the chemical is completely dissociated
Kd	Reference source : « Regional Screening Level » (RSLs) database (US-EPA)
Dpe	Reference source : Lijzen *et al*. (2001)

Parameters « Plants » (S-RISK WAL®)	**Recommendations**
BCF BioConcentration Factor (from soil to plant)	<u>For organic chemicals :</u> Specific information for Trapp's model[17] (used by S-RISK WAL®) Caution: the Trapp's equations are validated only for log Kow>1. If log Kow<1, the Briggs *et al.* equations (1982, 1983)[18] have to be used in the range -0.57<log Kow<3.7. If log Kow<-0.57, the selected value will be log Kow = -0.57. *BCF values (only 2 types of vegetables (root- and leafy-vegetable) from Briggs et al. relationships are set in S-RISK WAL® as follows :* - *root : « potatoes » / « roots and tuberous »/ « bulbous » ;* - *leafy: « cabbages »/ »leafy vegetables »/grasses / « fruit vegetables »/ « leguminous vegetables »/ « grain ».* <u>For inorganic chemicals :</u> Experimental values obtained in Walloon soils during POLLUSOL 2 study are preferred (400 soils and 1340 vegetables) for Al, Ba, Be, Co, Mo, Sb, Se, Sn and Mn (cf. Appendix 1). All POLLUSOL 2 data are free of charge and available upon request at SPAQuE (by e-mail to Julie LECLERCQ in charge of this project, j.leclercq@spaque.be). BCF values from POLLUSOL 2 study may be used in S-RISK WAL® as follows: - Potatoes : plant type « potatoes » ; - Carrots : plant types « roots and tuberous »/ « bulbous » ; - Lettuces : plant types « cabbages »/ « leafy vegetables »/ « grasses » ; - Beans: plant types « fruit vegetables »/ « leguminous vegetables »/ « grain ». When no experimental BCF could be identified, the regression model developed by Baes et al. (1984, A Review and Analysis of Parameters for Assessing Transport of Environmentally Released Radionuclides through Agriculture. ORNL-5786. Oak Ridge National Laboratory) could be used. Ln $BCF_{r/s}$ = 2.67 – 1.12 x Ln Kd BCFr/s : bioconcentration factor expressed as [$mg/kg_{plant\ dw}$]/[$mg/kg_{soil\ dw}$]

[17] Trapp, S. (2002). Dynamic root uptake model for neutral lipophilic organics. Environmental Toxicology and Chemistry, 21(1), 203-206.
Trapp, S., Cammarano, A., Capri, E., Reichenberg, F., & Mayer, P. (2007). Diffusion of PAH in potato and carrot slices and application for a potato model. Environmental Science & Technology, 41(9), 3103-3108.
Trapp, S., & Matthies, M. (1995). Generic one-compartment model for uptake of organic chemicals by foliar vegetation. Environmental Science & Technology, 29(9), 23332338.

[18] Briggs *et al*. (1982): « Relationships between lipophilicity and root uptake of non-ionised chemicals by Barley. Pestic. Sci. 13, 495-504 », Briggs, G.C., Bromilow, R.H. & Evans, A.A., *1982*
Briggs *et al.* (1983): « Relationship between lipophilicity and the distribution of non-ionised chemicals in Barley shoots following uptake by the roots. Pestic. Sci. (14), 492-500 », Briggs, G.C., Bromilow, R.H., Evans, A.A. & Williams, M. *1983*

	Where: $BCF_{r/s}$ is the *BioConcentration Factor calculated for both root and stem/leaf vegetables.* For other chemicals, values found in literature can be used (example: for PCB, Cullen et *al.*, 1996, reference source [7]). *If no data available, S-RISK WAL® will calculate the BCF values (« Use model »).*

Parameters in « Animals » file (S-RISK WAL®)	**Recommendations**
BTF	For organic chemicals: *Calculation done by S-RISK WAL® with equations based on log Kow (« Use model »).* For inorganic chemicals: Check in « Verification of radionuclide transfer factors to domestic-animal food products using indigenous elements and with emphasis on iodine », Sheppard *et al.*, 2010. If no data available, BTF = 0 by default, leading to a misestimated soil screening value for agricultural use.

Parameters In « Exposure » (S-RISK®)	**Recommendations**
Kp	For organic chemicals: First choice: experimental values in "Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment) - Exhibit B-2 – Kp measured") from US-EPA *Otherwise, the calculation will be done by S-RISK WAL® (« Use model »)* For inorganic chemicals: First choice: the value by default of 10^{-3} cm/h (cf. US EPA "Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment)).
ABS dermal, soil/dust	First choice 1: experimental values in "Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment) – US-EPA 2: values in tables "Regional Screening Levels (RSLs) – User's Guide » (US-EPA) 3: RAIS[19] database (https://rais.ornl.gov/), «Federal Contaminated

[19] RAIS, Risk Assessment Information System

	Site Risk Assessment in Canada, Part II: Health Canada Toxicological Reference Values (TRVs) and Chemical-Specific Factors, Version 2.0», *September 2010*). CAUTION : Do NOT select the value 0.1 for semi-volatile organics indicated in US EPA RAGS-E and RAIS. Set 0.25 by default if no data available.
FA	*<u>For organic chemicals:</u>* *After checking that FA is within the right range (with B et T_{event} calculated in S-RISK WAL®. Otherwise, this parameter has to be adjusted using the S-RISK WAL® user's manual (4.10.5 Dermal exposure parameters).* *If FA is not within the range in the graph $B=f(T_{event})$, selection of FA=1 by default.* *<u>For inorganic chemicals:</u>* *FA=1 by default (not possible to adjust in S-RISK WAL®).*

METHODOLOGY TO SELECT THE « DRINKING WATER CRITERIA » or « TAP WATER »

The Limit Value established for the protection of groundwater, **called VL_nappe in the table**, is similar to a « drinking water criteria » or a « tap water » screening value. This Limit value is appropriate for groundwater/aquifer used for the tap water production. This value is selected by following this priority order (going from regional level to international level):

1. **Walloon Water Regulation** « Code de l'Eau » – Appendix XIV (groundwater quality) and Appendix XXXI (drinking-water quality)
2. **Flanders Regulation (2007)**: Trigger values in the 14th of December 2007 Flemish Decree about soil protection and soil remediation
3. **Brussels Regulation (2018)** : Trigger values in the 29th of March 2018 Brussels Decree
4. **WHO (2017)** : Guidelines for drinking-water quality - 4th edition
5. **The Netherlands Regulation (2013) – Table 1** : Intervention Levels in the 27th of June 2013 "Circulaire Bodemsanering"
6. **US EPA (MCL)** : Maximum Contaminant Levels (MCL) in "Table of regulated drinking water contaminants"
7. **OEHHA (NL)** : Notification Levels (NL)
8. **US EPA (RSL)** – Tap water Screening Levels in "Regional Screening Levels – Generic tables"

9. **The Netherlands Regulation (2013) –Table 2** : Screening Levels of high pollution in the 27th of June 2013 "Circulaire Bodemsanering"

10. If no data available, the Guideline Value is calculated following the WHO's methodology for the drinking-water guidelines:

$$\text{Guideline Value (mg/L)} = \frac{\text{TRV (mg/kg bw·d) x BW (kg bw) x P (-)}}{\text{C (L/d)}}$$

Where (WHO's assumptions):
TRV: Toxicity Reference Value for oral exposure (mg/kg bw·d)
BW: body weight (60 kg by default)
P: fraction of the TRV allocated to drinking-water (20 %)
C: Daily drinking-water consumption (2 L/d)

Sometimes, the limit value could be weighted by factor. In this case, the factor should be indicated.

METHODOLOGY FOR THE CALCULATION OF VL_H WITH S-RISK® WAL (in Wallonia)

The Limit Values for the human health protection (VL_H) are calculated with S-RISK WAL®, (application I).

METHODOLOGY FOR THE CALCULATION OF $VL_{nappe[volatilisation]}$ and $VL_{nappe\_non\_exploitable}$

$VL_{nappe[volatilisation]}$

The $VL_{nappe[volatilisation]}$ screening levels, taking into account the volatilization of a volatile chemical in groundwater through the soil layer, are calculated with S-RISK WAL®, considering the following assumptions:

- the residential land use ;
- the limit value in groundwater for a hazard quotient of 1 and /or excess risk of 10^{-5} (the lowest VL will be selected at the end) ;
- the relevant exposure pathways: indoor inhalation (vapors), outdoor inhalation (vapors), inhalation of vapors during the shower.

NB : in case of $VL_{nappe[volatilisation]}$ below VL_{nappe}, $VL_{nappe[volatilisation]}$ is by default equal to VL_{nappe}.

VLnappe_non_exploitable :

This Limit value is appropriate for groundwater/aquifer not used for the tap water production.

After hydrogeology expert's consultation, these Limit Values have been estimated as twice the VL_{nappe} value.

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Appendix 1: BCF's equations established on the basis of POLLUSOL 2 database (400 soil samples and 1340 vegetable samples)

Sheet "Plants" >> Switch to Tier 2 >> Add or adjust available BCF models >> or

BCF = fill the box

log(BCF) = (fill the box) + log(Soil-conc) * (fill the box)

BCF_{dw} or log $(BCF)_{dw}$	Tuber vegetable	Root vegetables	Leaf vegetables	Fruit vegetables (e.g. bean)	Fruit vegetables (e.g. courgette)
Aluminium	BCF = 0,0004271	BCF = 0,001661	BCF = 0,01633	BCF = 0,001478	log(BCF) = (1,17) + log(Soil-conc) * (-1)
Antimony	log(BCF) = (-1,36) + log(Soil-conc) * (-1)	log(BCF) = (-1,04) + log(Soil-conc) * (-1)	log(BCF) = (-0,84) + log(Soil-conc) * (-1)	log(BCF) = (-0,83) + log(Soil-conc) * (-1)	log(BCF) = (-0,83) + log(Soil-conc) * (-1)
Arsenic	BCF = 0,006300	BCF = 0,01270	BCF = 0,04521	BCF = 0,009490	BCF = 0,012071
Baryum	log(BCF) = (0,64) + log(Soil-conc) * (-1)	BCF = 0,05768	BCF = 0,1177	BCF = 0,05196	log(BCF) = (1,17) + log(Soil-conc) * (-1)
Beryllium	log(BCF) = (-1,66) + log(Soil-conc) * (-1)	log(BCF) = (-1,34) + log(Soil-conc) * (-1)	log(BCF) = (-1,14) + log(Soil-conc) * (-1)	log(BCF) = (-1,13) + log(Soil-conc) * (-1)	log(BCF) = (-1,13) + log(Soil-conc) * (-1)
Cadmium	BCF = 0,07773	BCF = 0,2400	BCF = 0,6935	BCF = 0,06191	BCF = 0,1200
Chromium	log(BCF) = (-1,25) + log(Soil-conc) * (-1)	BCF = 0,008140	BCF = 0,04462	BCF = 0,009744	BCF = 0,01567
Cobalt	log(BCF) = (-1,36) + log(Soil-conc) * (-1)	log(BCF) = (-1,04) + log(Soil-conc) * (-1)	BCF = 0,05311	log(BCF) = (-0,83) + log(Soil-conc) * (-1)	log(BCF) = (-0,83) + log(Soil-conc) * (-1)
Copper	BCF = 0,1064	log(BCF) = (0,5632) + log(Soil-conc) * (-0,9496)	BCF = 0,2128	log(BCF) = (0,8384) + log(Soil-conc) * (-1,0377)	BCF = 0,2418
Lead	BCF = 0,001226	BCF = 0,003430	BCF = 0,01355	BCF = 0,002546	log(BCF) = (-0,83) + log(Soil-conc) * (-1)
Manganese	log(BCF) = (0,5028) + log(Soil-conc) * (-0,912)	BCF = 0,01097	BCF = 0,07230	BCF = 0,02370	BCF = 0,02430
Mercury	log(BCF) = (-2,06) + log(Soil-conc) * (-1)	log(BCF) = (-1,74) + log(Soil-conc) * (-1)	BCF = 0,1124	log(BCF) = (-1,53) + log(Soil-conc) * (-1)	log(BCF) = (-1,53) + log(Soil-conc) * (-1)
Molybdène	BCF = 0,5724	BCF = 0,3124	BCF = 1,3049	BCF = 3,1203	BCF = 1,2315
Nickel	BCF = 0,01018	BCF = 0,01810	BCF = 0,04797	BCF = 0,03663	BCF = 0,04575
Selenium	BCF = 0,1257	log(BCF) = (-0,74) + log(Soil-conc) * (-1)	BCF = 0,4604	BCF = 0,2252	log(BCF) = (-0,53) + log(Soil-conc) * (-1)
Tin	log(BCF) = (0,34) + log(Soil-conc) * (-1)	log(BCF) = (0,66) + log(Soil-conc) * (-1)	log(BCF) = (0,86) + log(Soil-conc) * (-1)	log(BCF) = (0,87) + log(Soil-conc) * (-1)	log(BCF) = (0,87) + log(Soil-conc) * (-1)
Zinc	log(BCF) = (0,6392) + log(Soil-conc) * (-0,7664)	BCF = 0,07432	BCF = 0,2636	log(BCF) = (1,3565) + log(Soil-conc) * (-0,896)	BCF = 0,1760

Data obtained by SPAQuE on 1341 samples of vegetables harvested in 398 vegetable gardens in urban areas near industry (Wallonia, Belgium)

Legend

most of C_{plant} > LQ, concentration in vegetable is strongly correlated with soil concentraton : regression

most of C_{plant} > LQ, concentration in vegetable weakly correlated with soil concentration : mean

at least 20 pairs (soil-plant) where C_{soil} and C_{plant} > LQ : mean

most of C_{plant} < LQ, BCF_{max} estimated by LQ/C_{soil})