HERisk Guide

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Summary

HUMAN HEALTH RISK

Equations used by HERisk for non-carcinogenic and carcinogenic risks calculations. These equations were taken from the U.S. EPA (2009a, 2004, 1989) guidelines. Some parameters used in these calculations are summarized in **Tables 6–8**.

Table 1 – Equations used by HERisk for doses or exposure concentration calculations

Description	Equation	Parameters used	Reference
Dose concentrations calculation			
Daily intake dose of chemical species by soil ingestion for initial age *IA* (mg kg^{-1} d^{-1})	$D_{ing\_s}{}^{IA}(t) = \sum_{t=\Delta t}^{ED} \frac{C_s(t) \cdot IR_s(i) \cdot CF_1 \cdot FI_s \cdot EF(i) \cdot \Delta t}{BW(i) \cdot AT}$ (1)	***C_s (t)*** = Chemical species concentration in soil at time *t* (mg kg^{-1}); ***IR_s (i)*** = Soil ingestion rate for age group *i* (mg d^{-1}); ***CF_1*** = Conversion factor (kg mg^{-1}); ***FI_s*** = Fraction ingested of contaminated soil; ***EF (i)*** = Exposure frequency for age group *i* (d y^{-1}); ***BW (i)*** = Body weight for age group *i* (kg); ***AT*** = Averaging time (d); ***Δt*** = Time variation (y); ***ED*** = Number of years of exposure duration.	U.S. EPA (1989)
Daily intake dose of chemical species by water ingestion for initial age *IA* (mg kg^{-1} d^{-1})	$D_{ing\_w}{}^{IA}(t) = \sum_{t=\Delta t}^{ED} \frac{C_w(t) \cdot IR_w(i) \cdot EF(i) \cdot \Delta t}{BW(i) \cdot AT}$ (2)	***C_w (t)*** = Chemical species concentration in water at time *t* (mg L^{-1}); ***IR_s (i)*** = Water ingestion rate for age group *i* (L d^{-1}).	U.S. EPA (1989)
Daily chemical species absorption dose by dermal contact with soil for initial age *IA* (mg kg^{-1} d^{-1})	$D_{der\_s}{}^{IA}(t) = \sum_{t=\Delta t}^{ED} \frac{C_s(t) \cdot CF_1 \cdot SA_s(i) \cdot AF(i) \cdot ABS \cdot EV_s(i) \cdot EF(i) \cdot \Delta t}{BW(i) \cdot AT}$ (3)	***SA_s (i)*** = Skin surface area available for contact with soil for age group *i* (cm^2); ***AF (i)*** = Soil adherence factor for age group *i* (mg cm^{-2} event^{-1}); ***ABS*** = Dermal absorption fraction; ***EV_s (i)*** = Event frequency for age group *i* (events d^{-1}).	U.S. EPA (2004)
Daily chemical species absorption dose by dermal contact with water for initial age *IA* (mg kg^{-1} d^{-1})	$D_{der\_w}{}^{IA}(t) = \sum_{t=\Delta t}^{ED} \frac{C_w(t) \cdot CF_3 \cdot SA_w(i) \cdot PC \cdot ET_w(i) \cdot EV_w(i) \cdot EF(i) \cdot \Delta t}{BW(i) \cdot AT}$ (4)	***CF_3*** = Volumetric conversion factor (L cm^{-3}); ***SA_w (i)*** = Skin surface area available for contact with water while swimming or showering for age group *i* (cm^2); ***PC*** = Dermal permeability of the chemical species (cm h^{-1}); ***ET_w (i)*** = Water exposure time while swimming or showering for age group *i* (h event^{-1}); ***EV_w (i)*** = Swimming or showering event frequency for age group *i* (events d^{-1}).	U.S. EPA (2004)

Description	Equation	Parameters used	Reference
Doses or exposure concentrations calculation			
Daily intake dose of chemical species by food ingestion for initial age *IA* (mg kg^{-1} d^{-1})	$D_{ing\_f}^{IA}(t) = \sum_{t=\Delta t}^{ED} \frac{C_f(t) \cdot IR_f(i) \cdot FI_f \cdot EF(i) \cdot \Delta t}{BW(i) \cdot AT}$ (5)	***C_f (t)*** = Chemical species concentration in food at time *t* (mg kg^{-1}); ***IR_f (i)*** = Food ingestion rate for age group *i* (mg d^{-1}); ***FI_f*** = Fraction ingested of contaminated food; ***EF (i)*** = Exposure frequency for age group *i* (d y^{-1}); ***BW (i)*** = Body weight for age group *i* (kg); ***AT =*** Averaging time (d); ***Δt*** = Time variation (y); ***ED*** = Number of years of exposure duration.	U.S. EPA (1989)
Exposure concentration for initial age *IA* (mg m^{-3})	$EC^{IA}(t) = \sum_{t=\Delta t}^{ED} \frac{C_{air}(t) \cdot ET_{inh}(i) \cdot EF(i) \cdot \Delta t}{AT_h}$ (6)	***C_{air} (t)*** = Chemical species concentration in steam or particulate matter at time *t* (mg m^{-3}); ***ET_{inh} (i)*** = Exposure time at age *i* (h d^{-1}); ***AT_h =*** Averaging time (h).	U.S. EPA (2009a)

In equation 5, the concentration of contaminants in the food (C_{food}) could be estimated from the concentration of contaminants in the soil (C_{soil}) and/or water (C_{water}), through Biotransfer factors (*BTF*) and others parameters. The *BTF* values are generally determined through bioassays and are available in the literature.

In agricultural areas, is common the presence of animals and vegetables that can be raised and cultivated in the interest contaminated areas. To assess all possible routes of humans' contamination, HERisk uses formulas for modeling the transport of contaminants present in soil and water to animals and vegetables which will later be ingested by humans. Some parameters used in these calculations are summarized in **Tables 9–10**.

Table 2 – Equations used by HERisk for modeling the transport of contaminants

Description	Equation	Parameters used	Reference
Modeling the transport of contaminants present in soil and water to bovine meat or milk			
Chemical species concentration in meat or milk derived from accidental soil ingestion by the cattle (mg kg^{-1})	$C_{M-1}(t) = C_s(t) \cdot BTF_{s-M} \cdot IR_{s-cattle} \cdot Fa \cdot Fp$ (7)	$\boldsymbol{BTF_{s\text{-}M}}$ = Biotransfer factor of the chemical species from soil to meat or milk (d kg^{-1}); $\boldsymbol{IR_{s\text{-}cattle}}$ = Soil ingestion rate by beef or dairy cattle (kg d^{-1}); ***Fa*** = Fraction of the site that is contaminated; ***Fp*** = Fraction of the year that the cattle remains on the site.	Health Canada (2005)
Chemical species concentration in meat or milk derived from water ingestion by the cattle (mg kg^{-1})	$C_{M-2}(t) = C_w(t) \cdot BTF_{w-M} \cdot IR_{w-cattle} \cdot fw$ (8)	$\boldsymbol{BTF_{w\text{-}M}}$ = Biotransfer factor of the chemical species from water to meat or milk (d kg^{-1}); $\boldsymbol{IR_{w\text{-}cattle}}$ is the water ingestion rate by beef or dairy cattle (L d^{-1}); ***fw*** = Daily fraction of consumed water that is contaminated.	Health Canada (2005)
Chemical species concentration in meat or milk derived from contaminated feed plants ingestion by the cattle (mg kg^{-1})	$C_{M-3}(t) = C_s(t) \cdot BTF_{s-f.p} \cdot CF_2 \cdot BTF_{f.p-M} \cdot IR_{f.p.-cattle} \cdot Fa \cdot Fp$ (9)	$\boldsymbol{BTF_{s\text{-}f.p.}}$ = Biotransfer factor of the chemical species from soil to feed plants; $\boldsymbol{CF_2}$ = Dry/wet weight adjustment (85% vegetable moisture); $\boldsymbol{BTF_{f.p.\text{-}M}}$ = Biotransfer factor of the chemical species from feed plants to meat or milk (d kg^{-1}); $\boldsymbol{IR_{f.p.\text{-}cattle}}$ is the feed plants ingestion rate by beef or dairy cattle (kg d^{-1}).	Health Canada (2005)

Description	Equation	Parameters used	Reference
Modeling the transport of contaminants present in soil and water to bovine meat or milk			
Total chemical species concentration in meat or milk (mg kg^{-1})	$C_{f-M}(t) = \sum_{\gamma=1}^{3} C_{M-\gamma}(t)$ (10)	***C**$_{M-\gamma}$* = Chemical species concentration in meat or milk derived from contaminated feed plants (mg kg^{-1}), water or soil (mg kg^{-1}).	Health Canada (2005)
Modeling the transport of contaminants present in soil to fruits, grains, seeds, tubers and vegetables			
Total chemical species concentration in fruits, grains, seeds, tubers or vegetables (mg kg^{-1})	$C_v(t) = C_s(t) \cdot BTF_{s-v} \cdot CF_2$ (11)	***BTF**$_{s-v}$* = Biotransfer factor of the chemical species from soil to fruits, grains, seeds, tubers or vegetables; ***CF**$_2$* = Dry/wet weight adjustment (85% vegetable moisture);	Health Canada (2005)
Modeling the transport of contaminants present in water to fish			
Total chemical species concentration in fish (mg kg^{-1})	$C_{fish}(t) = C_w(t) \cdot BTF_{w-fish}$ (12)	***BTF**$_{w-fish}$* = Biotransfer factor of the chemical species from water to fish;	Health Canada (2005)
Modeling the transport of contaminants present in soil and water to bird meat or eggs			
Chemical species concentration in bird meat or eggs derived from accidental soil ingestion by the bird (mg kg^{-1})	$C_{X-1}(t) = C_s(t) \cdot BTF_{s-X} \cdot IR_{s-X} \cdot Fa \cdot Fp$ (13)	***BTF**$_{s-X}$* = Biotransfer factor of the chemical species from soil to bird meat or eggs (d kg^{-1}); ***IR**$_{s-X}$* = Soil ingestion rate by bird (kg d^{-1}); ***Fa*** = Fraction of the site that is contaminated; ***Fp*** = Fraction of the year that the bird remains on the site.	Health Canada (2005)

Description	Equation	Parameters used	Reference
Modeling the transport of contaminants present in soil and water to bird meat or eggs			
Chemical species concentration in meat or eggs derived from accidental soil ingestion by the bird (mg kg^{-1})	$C_{X-1}\,(t)\ = C_s\,(t) \cdot BTF_{s-X} \cdot IR_{s-X} \cdot Fa\ \cdot Fp \qquad (13)$	***BTF**$_{s\text{-}X}$* = Biotransfer factor of the chemical species from soil to bird meat or eggs (d kg^{-1}); ***IR**$_{s\text{-}X}$* = Soil ingestion rate by bird (kg d^{-1}); ***Fa*** = Fraction of the site that is contaminated; ***Fp*** = Fraction of the year that the bird remains on the site.	Health Canada (2005)
Chemical species concentration in meat or eggs derived from water ingestion by the bird (mg kg^{-1})	$C_{X-2}\,(t)\ = C_w\,(t) \cdot BTF_{w-X} \cdot IR_{w-X} \cdot fw \qquad (14)$	***BTF**$_{w\text{-}X}$* = Biotransfer factor of the chemical species from water to bird meat or eggs (d kg^{-1}); ***IR**$_{w\text{-}X}$* is the water ingestion rate by bird (L d^{-1}); ***fw*** = Daily fraction of consumed water that is contaminated.	Health Canada (2005)
Total chemical species concentration in bird meat or eggs (mg kg^{-1})	$C_{f-X}\,(t)\ = \sum_{\gamma=1}^{2} C_{X-\gamma}\,(t) \qquad (15)$	***C**$_{X\text{-}\gamma}$* = Chemical species concentration in bird meat or eggs derived from contaminated water or soil (mg kg^{-1}).	Health Canada (2005)

Exposure to chemicals may cause carcinogenic and non-carcinogenic effects, which are treated differently in the risk assessment calculations. The carcinogenic effects are stochastic in nature and do not have a safe dose threshold, while the non-carcinogenic effects already appear after exceeding a certain dose threshold. The non-carcinogenic hazard quotient (*HQ*) and the potential carcinogenic risk (*CR*) are calculated using equations provided by U.S. EPA (2007, 2005a). Some parameters used in these calculations are summarized in **Tables 11–14**.

Table 3 – Equations used by HERisk for the calculation of non-carcinogenic hazard quotient and potential carcinogenic risk

Description	Equation	Parameters used	Reference
Non-carcinogenic hazard quotient (*HQ*)			
Non-carcinogenic hazard quotient for oral pathway and for initial age *IA*	$HQ_{oral}^{IA}(t) = \frac{D_{oral}^{IA}(t) \cdot BAF}{RfD_{oral}}$ (16)	$\boldsymbol{D_{oral}^{IA}}$ = Daily orally intake dose of chemical species for initial age *IA* (mg kg^{-1} d^{-1}); ***BAF*** = Chemical species dose fraction that are absorbed by the organism (bioavailability factor); $\boldsymbol{RfD_{oral}}$ = Reference oral dose of the chemical species (mg kg^{-1} d^{-1}).	U.S. EPA (2007)
Non-carcinogenic hazard quotient for dermal pathway and for initial age *IA*	$HQ_{dermal}^{IA}(t) = \frac{D_{dermal}^{IA}(t)}{RfD_{dermal}}$ (17)	$\boldsymbol{D_{dermal}^{IA}}$ = Daily absorbed dose of chemical species for initial age *IA* (mg kg^{-1} d^{-1}); $\boldsymbol{RfD_{dermal}}$ = Reference dermal dose of the chemical species (mg kg^{-1} d^{-1}); in this case ***BAF*** are already considered in the calculation of doses as ***PC*** or ***ABS***.	U.S. EPA (2007)
Non-carcinogenic hazard quotient for inhalation pathway and for initial age *IA*	$HQ_{inha.}^{IA}(t) = \frac{EC^{IA}(t) \cdot BAF}{RfC}$ (18)	$\boldsymbol{EC^{IA}}$ = Exposure concentration of chemical species for initial age *IA* (mg m^{-3}); ***BAF*** = Chemical species dose fraction that are absorbed by the organism (bioavailability factor); ***RfC*** = Reference concentration of the chemical species (mg m^{-3}).	U.S. EPA (2007)

Description	Equation	Parameters used	Reference
	Potential carcinogenic risk (*CR*)		
Potential carcinogenic risk for oral pathway and for initial age *IA*	$CR_{oral}^{IA}\ (t)\ = D_{oral}^{IA}(t) \cdot BAF \cdot SF_{oral} \cdot ADAF_{oral}$ (19)	$\boldsymbol{D_{oral}}^{\boldsymbol{IA}}$ = Daily orally intake dose of chemical species for initial age *IA* (mg kg^{-1} d^{-1}); ***BAF*** = Chemical species dose fraction that are absorbed by the organism (bioavailability factor); $\boldsymbol{SF_{oral}}$ = Oral slope factor of the chemical species (mg kg^{-1} d^{-1})$^{-1}$; $\boldsymbol{ADAF_{oral}}$ = Age dependent adjustments factors in case of chemical species has a mutagenic mode of action by oral intake.	U.S. EPA (2007, 2005a)
Potential carcinogenic risk for dermal pathway and for initial age *IA*	$CR_{dermal}^{IA}\ (t)\ = D_{dermal}^{IA}(t) \cdot SF_{dermal} \cdot ADAF_{dermal}$ (20)	$\boldsymbol{D_{dermal}}^{\boldsymbol{IA}}$ = Daily absorbed dose of chemical species for initial age *IA* (mg kg^{-1} d^{-1}); $\boldsymbol{SF_{dermal}}$ = Dermal slope factor of the chemical species (mg kg^{-1} d^{-1})$^{-1}$; $\boldsymbol{ADAF_{dermal}}$ = Age dependent adjustments factors in case of chemical species has a mutagenic mode of action by dermal absorption; in this case ***BAF*** are already considered in the calculation of doses as ***PC*** or ***ABS***.	U.S. EPA (2007, 2005a)
Potential carcinogenic risk for inhalation pathway and for initial age *IA*	$CR_{Inha.}^{IA}\ (t)\ = EC^{IA}\ (t) \cdot BAF \cdot IUR \cdot ADAF_{inha.}$ (21)	$\boldsymbol{EC}^{\boldsymbol{IA}}$ = Exposure concentration of chemical species for initial age *IA* (mg m^{-3}); ***BAF*** = Chemical species dose fraction that are absorbed by the organism (bioavailability factor); ***IUR*** = Inhalation Unit Risk of the chemical species (mg m^{-3})$^{-1}$; $\boldsymbol{ADAF_{inha.}}$ = Age dependent adjustments factors in case of chemical species has a mutagenic mode of action by inhalation intake.	U.S. EPA (2007, 2005a)

For carcinogen chemical species acting through a mutagenic Mode Of Action (MOA), where chemical-specific data concerning early life susceptibility are lacking, early life susceptibility should be assumed, and the following *ADAFs* (age dependent adjustments factors) should be applied to the cancer slope factor or the *IUR* as described in the U.S. EPA (2005a):

- *ADAF* = 10 for exposures occurring before 2 years of age;
- *ADAF* = 3 for exposures occurring between the ages of 2 and 16 years of age;
- *ADAF* = 1 (no adjustment) for exposures occurring after 16 years of age.

According to U.S. EPA (2009a), adults and children presents differences in the particle deposited dose in the entire respiratory tract. Several studies indicate differences in the deposition; however, values vary widely, and no correction values can be defined. Still according to U.S. EPA (2009a), considering that 100% of the deposited dose in the entire respiratory tract is available for uptake into the systemic circulation can circumvent the error caused by the particle deposition differences.

The risk assessment normally is performed with more than one exposure route (n), for this reason, it is necessary to calculate the aggregated hazard index (HI_{agg}), which is the sum of all calculated *HQ* for each exposure route. The same can be done for the carcinogenic risk by calculating the aggregated potential carcinogenic risk (CR_{agg}) (U.S. EPA, 1989).

For the final risk assessment, the sum of the risks arising from all exposure routes and from each chemical species (w) was calculated, obtaining the total hazard index (HI_{tot}) and the cumulative potential carcinogenic risk (CR_{cum}). The classifications of human health risks are shown in **Table 5**.

Table 4 – Equations used by HERisk for the calculation of risk indices and potential carcinogenic risks

Description	Equation	Parameters used	Reference
Human health risk assessment			
Calculation of risk indices and potential carcinogenic risks			
Aggregated hazard index for initial age *IA*	$HI_{agg}{}^{IA}(t) = \sum_{w=1}^{z} HQ_w(t)$ (22)	***HQ_w (t)*** = Hazard Quotient of route *w* at time *t*; ***z*** = Number of exposure routes.	U.S. EPA (1989)
Aggregated potential carcinogenic risk for initial age *IA*	$CR_{agg}{}^{IA}(t) = \sum_{w=1}^{z} CR_w(t)$ (23)	***CR_w (t)*** = Potential carcinogenic risk of route *w* at time *t*.	U.S. EPA (1989)
Total hazard index for initial age *IA*	$HI_{tot}{}^{IA}(t) = \sum_{j=1}^{n} HI_{agg,j}(t)$ (24)	***$HI_{agg,j}$*** = Aggregated Hazard Index of chemical species *j* at time *t*; ***n*** = Number of chemical species.	U.S. EPA (1989)
Cumulative potential carcinogenic risk for initial age *IA*	$CR_{cum}{}^{IA}(t) = \sum_{j=1}^{n} CR_{agg,j}(t)$ (25)	***$CR_{agg,j}$*** = Aggregated potential carcinogenic risk of chemical species *j* at time *t*;	U.S. EPA (1989)

Table 5 – Human health risk characterizations

Risk	Non-carcinogenic (U.S. EPA, 1989)	Carcinogenic (Li et al., 2014)
Negligible	$HI < 0.1$	$CR < 1.0E\text{-}6$
Low	$0.1 \leq HI < 1.0$	$1.0E\text{-}6 \leq CR < 1.0E\text{-}4$
Medium	$1.0 \leq HI < 4.0$	-
High	$4.0 \leq HI$	$1.0E\text{-}4 \leq CR$

Uncertainties

When evaluating the effects of pollutants on human health and ecosystems, assessing uncertainties is an essential issue because it highlights the implications and limitations of the risk assessment process (Dong et al., 2015; Sassi et al., 2007). According to the U.S. EPA (1989), there are three different approaches to the uncertainty analysis: quantitative, semi-quantitative and qualitative methods. The quantitative approach involves the assessment of uncertainties in the exposure parameters, which provides crucial information on the variability and sensitivity of the calculated results (U.S. EPA, 1996). For that reason, this method was implemented in the HERisk code following the International Organization for Standardization (ISO) standard procedure reported in the Guide for the Expression of Uncertainty in Measurements (ISO, 2004).

The standard uncertainty of the magnitudes ($\boldsymbol{\sigma_F}$) is calculated as a combination of the standard uncertainties of the involved parameters, as shown below:

$$\sigma_F = \sqrt{\left(\sum_{i=1}^{N} \left(\frac{\partial F}{\partial x_i}\right)^2 \cdot \sigma^2(x_i)\right)} \qquad (26)$$

For example, in the absorbed doses (see Eqs. 1-6): x_i is the *i*th exposure parameter involved in each case, $\sigma(x_i)$ represents the standard uncertainty of the *i*th parameter, and the $(\partial F/\partial x_i)$ is the partial derivate by the *i*th variable, also known as sensitivity coefficients ($c(x_i)$).

Unfortunately, the risk calculations depend to a large extent on the quality of the database, which in general tends to be imprecise due to the high heterogeneity among the studies. The uncertainties $\sigma(x_i)$ of each exposure parameter, used in the HERisk code, were evaluated from all the information available in the specialized literature. In some cases, uncertainties were calculated from the statistical distribution functions reported for some parameters (Sassi et al., 2007; U.S. EPA, 1996). When there was no specific data available on the statistical distribution or the uncertainty of the parameter, 10% of this value was considered as its uncertainty. Due to, Averaging Time (*AT*) is not considered affected by variability, its uncertainty was considered null (Sassi et al., 2007).

Table 6 – Some parameters used in the calculations of doses

Symbol	Currently recommended value									Reference
	1 to <2 years	**2 to <3 years**	**3 to <6 years**	**6 to <11 years**	**11 to <16 years**	**16 to <18 years**	**18 to <21 years**	**21 to <65 years**	**>65 years**	
ABS	Chemical-specific value									Page 26
AF_{soil} (mg cm^{-2}) [a]	0.2140	0.2140	0.2140	0.1640	0.1640	0.1640	0.3745 0.6264 (Worker)	0.3745 0.6264 (Worker)	0.3745 0.6264 (Worker)	U.S. EPA (2011)
AT (d)	78 y · 365 d y^{-1} = 28,470 d (Carcinogenic effects) Δt (y) · 365 d y^{-1} (Non-carcinogenic effects)									U.S. EPA (2011)
AT_h (h)	78 y · 365 d y^{-1} · 24 h d^{-1} = 683,280 h (Carcinogenic effects) Δt (y) · 365 d y^{-1} · 24 h d^{-1} (Non-carcinogenic effects)									U.S. EPA (2011)
BW (kg)	11.4	13.8	18.6	31.8	56.8	71.6	71.6	80.0	80.0	U.S. EPA (2011)
C_{air} (mg m^{-3})	Site-specific value									-
C_{soil} (mg kg^{-1})	Site-specific value									-
C_{water} (mg L^{-1})	Site-specific value									-
CF_1 (kg mg^{-1})	$1 \cdot 10^{-6}$									U.S. EPA (2004)
CF_2 (L cm^{-3})	$1 \cdot 10^{-3}$									U.S. EPA (2004)
ED (y)										U.S. EPA (2011) U.S. EPA (1991)
EF (d y^{-1})	350 (Agricultural and residential scenario) 250 (Worker)									U.S. EPA (1991)
ET (h d^{-1})	24 (agricultural and residential) 8 (Worker)									Health Canada (2004)
ET_W (h d^{-1}) [c]	0.533	0.750	1.000	0.767	0.717	1.000	1.000	0.283	0.283	U.S. EPA (2011)
EV (events d^{-1})	1									U.S. EPA (2004)
FI	1									U.S. EPA (2011)

Continue

Continuation

Symbol		Currently recommended value									Reference
		1 to <2 years	**2 to <3 years**	**3 to <6 years**	**6 to <11 years**	**11 to <16 years**	**16 to <18 years**	**18 to <21 years**	**21 to <65 years**	**>65 years**	
IR_s (mg d^{-1})		100	100	200	100	100	100	100	50	50	U.S. EPA (2011)
		Agricultural scenario									
IR_f (kg d^{-1}) [d]	*Veg.*	0.1596	0.1932	0.2232	0.2576	0.3238	0.4081	0.4081	0.4560	0.4880	U.S. EPA (2011)
	Fruit	0.1037	0.1256	0.1265	0.1113	0.06816	0.08592	0.08592	0.1040	0.1680	
	Fish [e]	0.01824	0.02208	0.02976	0.04452	0.05680	0.07160	0.07160	0.1040	0.1120	
	Meat	0.06840	0.08280	0.1116	0.1336	0.1761	0.2220	0.2220	0.2240	0.1760	
	Milk	1.0488	1.2696	1.0788	1.0812	0.7952	1.0024	1.0024	0.6640	0.6400	
	Grain	0.1414	0.1711	0.2065	0.2608	0.2840	0.3580	0.3580	0.3680	0.2800	
		Residential scenario									
	Veg.	0.1778	0.2153	0.2771	0.2767	0.1988	0.2506	0.2506	0.2960	0.3520	
	Fruit	0.2428	0.2939	0.2492	0.3307	0.3124	0.3938	0.3938	0.4720	0.4880	
	Meat	0.1140	0.1380	0.1581	0.2035	0.2670	0.3365	0.3365	0.3280	0.2480	
	Milk	1.1138	1.3483	0.9504	1.0112	0.9315	1.1742	1.1742	0.8240	0.7680	
IR_w (L d^{-1})		0.837	0.877	0.959	1.316	1.821	1.783	2.368	2.958	2.730	U.S. EPA (2011)
PC (cm h^{-1})		Chemical-specific value									Page 28
SA_s (cm^2) [f]		6.10E+3	7.00E+3	9.50E+3	1.48E+4	2.06E+4	2.33E+4	2.33E+4	2.43E+4 [g]	2.26E+4 [h]	U.S. EPA (2011)
SA_w (cm^2) [f]		6.10E+3	7.00E+3	9.50E+3	1.48E+4	2.06E+4	2.33E+4	2.33E+4	2.43E+4 [g]	2.26E+4 [h]	U.S. EPA (2011)

All values taken from U.S. EPA (2011) are "per capita, 95th percentile"; [a] – Sum of skin area of face, arms, hands, legs and feet; [b] – Until reach average life expectancy; [c] – Bathing time; [d] – Intake rate in mg kg^{-1} day^{-1} multiplied by the weight of each age category. Both values were taken from U.S. EPA (2011); [e] – Intake rate of Fin fish and Shell fish; [f] – According to U.S. EPA (2011), 100% of skin area should be considered for contact with soil and water; [g] – Mean of values provided for adults and women between 21 and 60 years; [h] – Mean of values provided for adults and women over 60 years.

Table 7 – Some recommended values of dermal absorption fraction (*ABS*) from soil used for dose calculations

Chemical species	Dermal Absorption Fraction (ABS)[1]	Reference
Aluminum	0.10	Michigan DEQ (2015)
Antimony	0.10	Health Canada (2004)
Arsenic	0.03	Health Canada (2004); U.S. EPA (2004)
Barium	0.10	Health Canada (2004)
Cadmium	0.14	
Chromium (III)	0.04	
Chromium (VI)	0.09	
Cobalt	0.10	
Copper	0.10	
Iron	0.010	Michigan DEQ (2015)
Lead	0.006	Health Canada (2004)
Lithium	0.010	Michigan DEQ (2015)
Manganese	0.01	Michigan DEQ (2015)
Mercury	0.05	Health Canada (2004)
Nickel	0.35	
Silver	0.25	
Selenium	0.002	
Uranium	0.001	Craft et al. (2004)
Vanadium	0.10	Health Canada (2004)
Zinc	0.20	
Acenaphthene	0.20	
Acenaphthylene	0.18	
Acetophenone	0.10	Michigan DEQ (2015)
Anthracene	0.29	Health Canada (2004)
Benzo[*a*]anthracene	0.20	
Benzo[*a*]pyrene	0.20	
Benzo[*a*]pyrene and other PAHs	0.13	U.S. EPA (2004)
Benzo[*b*]fluoranthene	0.20	Health Canada (2004)
Benzo[*ghi*]perylene	0.18	
Benzo[*k*]fluoranthene	0.20	
Chrysene	0.20	
Dibenzo[*a*,*h*]anthracene	0.09	
Fluoranthene	0.20	
Fluorene	0.20	
Indeno[1,2,3-*cd*]pyrene	0.20	Health Canada (2004)
Naphthalene	0.10	Health Canada (2004)
Phenanthrene	0.18	
Pyrene	0.20	
Semivolatile organic compounds	0.10	U.S. EPA (2004)

[1] The values presented are experimental mean values.

The chemical species present in the database and not considered in the table, their values were considered as 0.13 if they are PAH (U.S. EPA (2004)) or 0.10 if they are PAH derivatives (considered as Semivolatile organic compounds, U.S. EPA (2004)).

The uncertainty values not reported in the table correspond to 10% of the parameter value.

Table 8 – Some permeability coefficients (*PC*) values used for dose calculations

Chemical species	Permeability Coefficient CP ($cm\ hr^{-1}$)	Reference
Inorganic chemical species		
Cadmium	1×10^{-3}	U.S. EPA (2004)
Chromium (VI)	2×10^{-3}	
Chromium (III)	1×10^{-3}	
Cobalt	4×10^{-4}	
Lead	1×10^{-4}	
Mercury(II)	1×10^{-3}	
Methyl mercury	1×10^{-3}	
Mercury vapor	2.4×10^{-1}	
Nickel	2×10^{-4}	
Potassium	2×10^{-3}	
Silver	6×10^{-4}	
Zinc	6×10^{-4}	
All other inorganics	1×10^{-3}	
Organic chemical species		
p-Benzoquinone	-	-
Acetophenone	-	-
Naphthalene	4.7×10^{-2}	U.S. EPA (2004)
Naphthoquinone	-	-
Acenaphthylene	-	-
Acenaphthene	$6.33 \times 10^{-3} \pm 4.81 \times 10^{-3}$	Sartorelli et al. (1998)
Fluorene	$6.26 \times 10^{-3} \pm 4.74 \times 10^{-3}$	Sartorelli et al. (1998)
2-Nitrobiphenyl *	3.8×10^{-2}	U.S. EPA (2004)
Phenanthrene	1.4×10^{-1}	U.S. EPA (2004)
Anthracene	$3.44 \times 10^{-3} \pm 3.09 \times 10^{-3}$	Sartorelli et al. (1998)
5-Nitroacenaphthene	-	-
Fluoranthene	2.2×10^{-1}	U.S. EPA (2004)
2-Nitrofluorene	-	-
Pyrene	$1.69 \times 10^{-3} \pm 1.36 \times 10^{-3}$	Sartorelli et al. (1998)
9,10-Phenanthrenequinone	-	-
Retene	-	-
9-Nitrophenanthrene	-	-
9-Nitroantracene	-	-
Benzo[*a*]fluorenone	-	-
Benz[*a*]anthracene	4.7×10^{-1}	U.S. EPA (2004)
Chrysene	4.7×10^{-1}	U.S. EPA (2004)
1-Nitropyrene	-	-
Benzo[*b*]fluoranthene	7.0×10^{-1}	U.S. EPA (2004)
Benzo[*k*]fluoranthene	-	-
Benzo[*e*]pyrene	-	-
Benzo[*a*]pyrene	7.0×10^{-1}	U.S. EPA (2004)
6H-Benzo[cd]pyren-6-one	-	-
Indeno[1,2,3-*cd*]pyrene	1.0	U.S. EPA (2004)
6-Nitrobenzo[a]pyrene	-	-
Dibenz[*a*,*h*]anthracene	1.5	U.S. EPA (2004)
Benzo[*ghi*]perylene	-	-

Table 9 – Some *BTF* values used in the transport modeling

BTF	Al	Cd	Pb	Co	Fe	Mn	Se	Zn	Cu	Ni
Ingestion to bovine meat [a] ***(day kg^{-1})*** *Reference:* Baes III et al. (1984)	1.50E-3	5.50E-4	3.00E-4	2.00E-2	2.00E-2	4.00E-4	1.50E-2	1.00E-1	1.00E-2	6.00E-3
Ingestion to bovine milk [a] ***(day kg^{-1})*** *Reference:* Baes III et al. (1984)	2.00E-4	1.00E-3	2.50E-4	2.00E-3	2.50E-3	3.50E-4	4.00E-3	1.00E-2	1.50E-3	1.00E-3
Soil to vegetative portions of food crops and feed plants *Reference:* Baes III et al. (1984)	4.00E-3	5.50E-1	4.50E-2	2.00E-2	4.00E-3	2.50E-1	2.50E-2	1.50E+0	4.00E-1	6.00E-2
Water to vegetative portions of food crops and feed plants *Reference:* [b]	4.00E-3	5.50E-1	4.50E-2	2.00E-2	4.00E-3	2.50E-1	2.50E-2	1.50E+0	4.00E-1	6.00E-2
Soil to nonvegetative (reproductive) portions of food crops and feed plants *Reference:* Baes III et al. (1984)	6.50E-4	1.50E-1	9.00E-3	7.00E-3	1.00E-3	5.00E-2	2.50E-2	9.00E-1	2.50E-1	6.00E-2
Water to nonvegetative (reproductive) portions of food crops and feed plants *Reference:* [c]	6.50E-4	1.50E-1	9.00E-3	7.00E-3	1.00E-3	5.00E-2	2.50E-2	9.00E-1	2.50E-1	6.00E-2

Continue

Continuation

BTF	As	Ba	Br	Cr(III)	Cr(VI)	U	V
Ingestion to bovine meat [a] ***(day kg^{-1})*** *Reference:* Baes III et al. (1984)	2.00E-3	1.50E-4	2.50E-2	5.50E-3	5.50E-3	2.00E-4	2.50E-3
Ingestion to bovine milk [a] ***(day kg^{-1})*** *Reference:* Baes III et al. (1984)	6.00E-5	3.50E-4	2.00E-2	1.50E-3	1.50E-3	6.00E-4	2.00E-5
Soil to vegetative portions of food crops and feed plants *Reference:* Baes III et al. (1984)	4.00E-2	1.50E-1	1.50E+0	7.50E-3	7.50E-3	8.50E-3	5.50E-3
Water to vegetative portions of food crops and feed plants *Reference:* [b]	4.00E-2	1.50E-1	1.50E+0	7.50E-3	7.50E-3	8.50E-3	5.50E-3
Soil to nonvegetative (reproductive) portions of food crops and feed plants *Reference:* Baes III et al. (1984)	6.00E-5	1.50E-2	1.50E+0	4.50E-3	4.50E-3	4.00E-3	3.00E-3
Water to nonvegetative (reproductive) portions of food crops and feed plants *Reference:* [c]	6.00E-5	1.50E-2	1.50E+0	4.50E-3	4.50E-3	4.00E-3	3.00E-3

[a] In the reference Baes III et al. (1984) *BTF* for cattle meat and milk does not depend on the type of matrix ingested by the animal (water, soil or food);

[b] It was assumed that *BTF* values for water to vegetative portions of food crops and feed plants are equal to *BTF* values for soil to vegetative portions of food crops and feed plants;

[c] It was assumed that *BTF* values for water to nonvegetative (reproductive) portions of food crops and feed plants are equal to *BTF* values for soil to nonvegetative (reproductive) portions of food crops and feed plants;

The uncertainty values not reported in the table correspond to 10% of the parameter value.

Table 10 – Some parameters values used in the transport modeling

Parameters	***Value***	**Reference**
$IR_{Water–beef\ cattle}$ (L day^{-1})	50.0	Health Canada (2005)
$IR_{Water–dairy\ cattle}$ (L day^{-1})	90.0	Health Canada (2005)
$IR_{soil–cattle}$ (kg day^{-1})	0.99	Health Canada (2005)
$IR_{feed\ plant–beef\ cattle}$ (kg day^{-1})	7.2	Health Canada (2005)
$IR_{feed\ plant–dairy\ cattle}$ (kg day^{-1})	16.1	Health Canada (2005)
CF_3	0.15	U.S. EPA (1998)
Fp	1.00	[a]
Fa	1.00	[a]

[a] The default value will consider that the entire fraction of water ingested is contaminated.

The uncertainty values not reported in the table correspond to 10% of the parameter value.

Table 11 – Some reference values used in the risk calculations

Chemical species	Oral *RfD*	Ref.	*RfC*	Ref.	Oral *SF*	Ref.	IUR	Ref.	Dermal *RfD **	Dermal *SF ***
p-Benzoquinone	n.a.	#	n.a.	#	n.a.	#	n.a.	#	n.a.	n.a.
Acetophenone	1.00E-1	IRIS/EPA (2020)	3.20E+0	Michigan DEQ (2015)	n.a.	#	n.a.	#	5.00E-2	n.a.
Naphthalene	2.00E-1	IRIS/EPA (2020)	3.00E-3	IRIS/EPA (2020)	1.20E-1 ± 1.03E-2	OEHHA (2019a)	3.4E-2	OEHHA (2019a)	1.78E-2	1.35E-1 ± 1.16E-2
1,4-Naphthoquinone	n.a.	#	n.a.	#	n.a.	#	n.a.	#	n.a.	n.a.
Acenaphthylene	6.00E-2	Michigan DEQ (2015)	2.1E-1	Michigan DEQ (2015)	n.a.	#	n.a.	#	5.34E-2	n.a.
Acenaphthene	6.00E-2	IRIS/EPA (2020)	2.1E-1	Michigan DEQ (2015)	n.a.	#	n.a.	#	5.34E-2	n.a.
Fluorene	4.00E-2	IRIS/EPA (2020)	1.4E-1	Michigan DEQ (2015)	n.a.	#	n.a.	#	3.56E-2	n.a.
2-Nitrobiphenyl	n.a.	#	n.a.	#	n.a.	#	n.a.	#	n.a.	n.a.
Phenanthrene	3.00E-2	Michigan DEQ (2015)	1.00E-4	Michigan DEQ (2015)	2.30E-3 ± 1.98E-4	Health Canada (2004)	3.10E-5	Health Canada (2004)	2.67E-2	2.58E-3 ± 2.23E-4
Anthracene	3.00E-1	IRIS/EPA (2020)	1.20E+0	OEHHA (2019b)	2.30E-1 ± 1.98E-2	Health Canada (2004)	3.10E-3	Health Canada (2004)	2.67E-1	2.58E-1 ± 2.23E-2
5-Nitroacenaphthene	n.a.	#	n.a.	#	1.30E-1 ± 1.12E-2	OEHHA (2019a)	3.70E-2	OEHHA (2019a)	n.a	2.60E-1 ± 2.24E-2
Fluoranthene	4.00E-2	IRIS/EPA (2020)	1.40E-1	Michigan DEQ (2015)	2.30E-3 ± 1.98E-4	Health Canada (2004)	3.10E-5	Health Canada (2004)	3.56E-2	2.58E-3 ± 2.23E-4
2-Nitrofluorene	n.a.	#	n.a.	#	1.20E-1 ± 1.04E-2	OEHHA (2019a)	1.10E-1	OEHHA (2019a)	n.a.	2.40E-1 ± 2.07E-2
Pyrene	3.00E-2	IRIS/EPA (2020)	1.20E-1	OEHHA (2019b)	n.a.	#	n.a.	#	2.67E-2	n.a.
9,10-Phenanthrenequinone	n.a.	#	n.a.	#	n.a.	#	n.a.	#	n.a.	n.a.
Retene	n.a.	#	n.a.	#	n.a.	#	n.a.	#	n.a.	n.a.
9-Nitrophenanthrene	n.a.	#	n.a.	#	n.a.	#	n.a.	#	n.a.	n.a.
9-Nitroantracene	n.a.	#	n.a.	#	n.a.	#	n.a.	#	n.a.	n.a.
Benzo[*a*]fluorenone	n.a.	#	n.a.	#	n.a.	#	n.a.	#	n.a.	n.a.
Benz[*a*]anthracene	n.a.	#	n.a.	#	2.30E-1 ± 1.98E-2	Health Canada (2004)	3.10E-3	Health Canada (2004)	n.a.	2.58E-1 ± 2.23E-2
Chrysene	n.a.	#	n.a.	#	2.30E-1 ± 1.98E-2	Health Canada (2004)	3.10E-3	Health Canada (2004)	n.a.	2.58E-1 ± 2.23E-2

Chemical species	Oral *RfD*	Ref.	*RfC*	Ref.	Oral *SF*	Ref.	IUR	Ref.	Dermal *RfD* *	Dermal *SF* **
1-Nitropyrene	n.a.	#	n.a.	#	1.20E+0 ± 1.04E-1	OEHHA (2019a)	1.10E-1	OEHHA (2019a)	n.a.	2.40E+0 ± 2.07E-1
Benzo[*b*]fluoranthene	n.a.	#	n.a.	#	2.30E-1 ± 1.98E-2	Health Canada (2004)	3.10E-3	Health Canada (2004)	n.a.	2.58E-1 ± 2.23E-2
Benzo[*k*]fluoranthene	n.a.	#	n.a.	#	2.30E-1 ± 1.98E-2	Health Canada (2004)	3.10E-3	Health Canada (2004)	n.a.	2.58E-1 ± 2.23E-2
Benzo[*e*]pyrene	n.a.	#	n.a.	#	n.a.	#	n.a.	#	n.a.	n.a.
Benzo[*a*]pyrene	3.00E-4	IRIS/EPA (2020)	2.00E-6	IRIS/EPA (2020)	1.00E+0 ± 8.63E-2	IRIS/EPA (2020)	6.00E-1	IRIS/EPA (2020)	2.67E-4	1.12E+0 ± 9.66E-2
6H-Benzo[*cd*]pyren-6-one	n.a.	#	n.a.	#	n.a.	#	n.a.	#	n.a.	n.a.
Indeno[1,2,3-*cd*]pyrene	n.a.	#	n.a.	#	2.30E-1 ± 1.98E-2	Health Canada (2004)	3.10E-3	Health Canada (2004)	n.a.	2.58E-1 ± 2.23E-2
6-Nitrobenzo[*a*]pyrene	n.a.	#	n.a.	#	n.a.	#	n.a.	#	n.a.	n.a.
Dibenz[*a*,*h*]anthracene	n.a.	#	n.a.	#	2.30E-1 ± 1.98E-2	Health Canada (2004)	3.10E-3	Health Canada (2004)	n.a.	2.58E-1 ± 2.23E-2
Benzo[*ghi*]perylene	2.00E-3	Michigan DEQ (2015)	7.00E-3	Michigan DEQ (2015)	2.30E-2 ± 1.98E-3	Health Canada (2004)	3.10E-4	Health Canada (2004)	1.78E-3	2.58E-2 ± 2.23E-3
Anthraquinone	2.00E-3	U.S. EPA (2011)	n.a.	#	4.00E-2 ± 3.45E-3	U.S. EPA (2011)	n.a.	#	1.00E-3	8.00E-2 ± 6.90E-3
6-Nitrochrysene	n.a.	#	n.a.	#	1.20E+2 ± 1.04E+1	OEHHA (2019a)	1.10E+1	OEHHA (2019a)	n.a.	2.40E+2 ± 2.08E+1
3-Nitrobenzanthrone	n.a.	#	n.a.	#	n.a.	#	n.a.	#	n.a.	n.a.
Pb	3.60E-3	Health Canada (2010)	1.50E-4	Michigan DEQ (2015)	8.50E-3 ± 7.33E-4	OEHHA (2019a)	1.20E-2	OEHHA (2019a)	3.60E-3	8.50E-3 ± 7.33E-4
Fe	7.00E-1	U.S. EPA (2006)	n.a.	#	n.a.	#	n.a.	#	7.0E-1	n.a.
Zn	3.00E-1	IRIS/EPA (2020)	1.20E-2	RIVM (2001)	n.a.	#	n.a.	#	n.a.	n.a.
Al	1.00E+0	ATSDR (2018)	5.50E-3	Michigan DEQ (2015)	n.a.	#	n.a.	#	1.00E+0	n.a.
Ba	2.00E-1	IRIS/EPA (2020)	5.00E-3	Michigan DEQ (2015)	n.a.	#	n.a.	#	1.40E-2	n.a.
Cu	1.00E-2	ATSDR (2018)	2.00E-3	Michigan DEQ (2015)	n.a.	#	n.a.	#	5.7E-3	n.a.
Cr(III)	1.50E+0	IRIS/EPA (2020)	5.00E-3	ATSDR (2018)	n.a.	#	1.09E+1	Health Canada (2010)	1.95E-2	n.a.
Cr(VI)	3.00E-3	IRIS/EPA (2020)	1.00E-4	IRIS/EPA (2020)	5.00E-1 ± 4.31E-2	OEHHA (2011)	1.20E+1	IRIS/EPA (2020)	7.50E-5	2.00E+1 ± 1.73E+0
Se	5.00E-3	IRIS/EPA (2020)	2.00E-2	Michigan DEQ (2015)	n.a.	#	n.a.	#	1.50E-3	n.a.

Chemical species	**Oral *RfD***	**Ref.**	***RfC***	**Ref.**	**Oral *SF***	**Ref.**	**IUR**	**Ref.**	**Dermal *RfD* ***	**Dermal *SF* ****
Ag	5.00E-3	IRIS/EPA (2020)	3.00E-3	Michigan DEQ (2015)	n.a.	#	n.a.	#	4.00E-2	n.a.
Sb	4.00E-4	IRIS/EPA (2020)	3.00E-4	ATSDR (2018)	n.a.	#	n.a.	#	6.00E-5	n.a.
U	3.00E-3	IRIS/EPA (2020)	8.00E-4	ATSDR (2018)	n.a.	#	n.a.	#	3.00E-3	n.a.
Mn	1.40E-1	IRIS/EPA (2020)	5.00E-5	IRIS/EPA (2020)	n.a.	#	n.a.	#	8.40E-3	n.a.
Cd	5.00E-4 (water) 1.00E-3 (food)	IRIS/EPA (2020)	1.00E-5	ATSDR (2018)	n.a.	#	1.80E+0	IRIS/EPA (2020)	2.50E-5 (water and food)	n.a.
As	3.00E-4	IRIS/EPA (2020)	1.50E-5	OEHHA (2019b)	1.50E+0 ± 1.29E-1	IRIS/EPA (2020)	4.30E+0	IRIS/EPA (2020)	2.85E-4	1.58E+0 ± 1.36E-1
Co	3.00E-4	U.S. EPA (2008a)	6.00E-6	U.S. EPA (2008a)	n.a	#	9.00E+0	Michigan DEQ (2015)	3.00E-4	n.a.
Hg	3.00E-4	Michigan DEQ (2015)	3.00E-4	IRIS/EPA (2020)	n.a	#	n.a	#	2.1E-5	n.a.
Ni	2.00E-2	IRIS/EPA (2020)	9.00E-5	ATSDR (2018)	n.a.	#	2.60E-1	OEHHA (2019a)	8.00E-4	n.a.
V	7.00E-5	U.S. EPA (2009b)	1.00E-4	ATSDR (2018)	n.a	#	n.a	#	1.82E-6	n.a.
Li	2.00E-3	U.S. EPA (2008b)	3.50E-2	Michigan DEQ (2015)	n.a	#	n.a	#	2.00E-3	n.a.
Br	1.00E+0	Public Health England (2009)	-	-	-	-	-	-	-	-

 # - No values were found in the literature (see database consulted in next page);
* - Value calculated by $RfD_{oral} \cdot ABS_{GI}$ as suggested by U.S. EPA (2004). ABS_{GI} values present in Table 10;
** - Value calculated by SF_{oral} / ABS_{GI} as suggested by U.S. EPA (2004). ABS_{GI} values present in Table 10;
n.a. – Not available

The uncertainty values not reported in the table correspond to 10% of the parameter value.

Database consulted:

(In order of preference for choosing *RfD* and *SF* values)

1. IRIS/USEPA - Integrated Risk Information System - U.S. Environmental Protection Agency;
2. ATSDR - Agency for toxic substances and disease registry;
3. Health Canada - Federal Contaminated Site Risk Assessment in Canada;
4. Michigan DEQ - Department of Environmental Quality - State of Michigan;
5. OEHHA - Office of Environmental Health Hazard Assessment.

Table 12 – Some recommended Gastrointestinal Absorption Fraction (*ABS_{GI}*) values used for the dermal reference values

Chemical species	***ABS_{GI}***	**Reference**
Sb	0.15	U.S. EPA (2004)
As	0.95	
Ba	0.07	
Be	0.007	
Cd	0.025 (food) 0.05 (water)	
Cr(III)	0.013	
Cr(VI)	0.025	
Mn	0.04	
Hg (soluble salts)	0.07	
Hg (metallic or insoluble)	0.74 – 0.80	
Ni	0.04	
Se	0.30 – 0.80	
Ag	0.04	
Tl	1.00	
V	0.026	
Zn	Highly variable	
Chlordane	0.80	
2,4-Dichlorophenoxyacetic acid (2,4-D)	> 0.90	
DDT	0.70 – 0.90	
Pentachlorophenol	0.76 (food) 1.00 (water)	
Polychlorinated biphenyls (PCBs)	0.80 – 0.96	
Polycyclic aromatic hydrocarbons (PAHs)	0.89	
TCDD	0.50 – 0.70	
Other Dioxins/Dibenzofurans	> 0.50	
All other organic compounds	Generally > 0.50	

According to U.S. EPA (2004), for those organic or inorganic chemicals that do not appear on the table above, the recommendation is to assume a 1.00 (100%) *ABS_{GI}* value.

Table 13 – Some *BAF* values used in the risk calculations

<table>
<tr><th rowspan="3">Chemical species</th><th colspan="12">BAF [a]</th></tr>
<tr><th colspan="10">Ingestion</th><th colspan="2">Inhalation</th></tr>
<tr><th>Soil</th><th>Water</th><th>Vegetable</th><th>Fruit</th><th>Beef</th><th>Milk</th><th>Bird</th><th>Egg</th><th>Fish</th><th>Grain</th><th>Part. matter</th><th>Steam</th></tr>
<tr><td>p-Benzoquinone</td><td colspan="10">1.000</td><td colspan="2">1.000</td></tr>
<tr><td>Reference</td><td colspan="10">b</td><td colspan="2">b</td></tr>
<tr><td>Acetophenone</td><td colspan="10">1.000 [c]</td><td colspan="2">1.000</td></tr>
<tr><td>Reference</td><td colspan="10">Michigan DEQ (2015)</td><td colspan="2">Health Canada (2004)</td></tr>
<tr><td>Naphthalene</td><td>1.000</td><td colspan="9">0.760 [d]</td><td colspan="2">1.000</td></tr>
<tr><td>Reference</td><td>Ehlers et al. (2003)</td><td colspan="9">Ramesh (2004)</td><td colspan="2">b</td></tr>
<tr><td>1,4-Naphthoquinone</td><td colspan="10">1.000</td><td colspan="2">1.000</td></tr>
<tr><td>Reference</td><td colspan="10">b</td><td colspan="2">b</td></tr>
<tr><td>Acenaphthylene</td><td>0.180</td><td colspan="9">0.890 [c]</td><td>0.442</td><td>1.000</td></tr>
<tr><td>Reference</td><td>Ehlers et al. (2003)</td><td colspan="9">U.S. EPA (2004)</td><td>Li et al. (2019)</td><td>b</td></tr>
<tr><td>Acenaphthene</td><td>0.180</td><td colspan="9">0.890 [c]</td><td>0.316</td><td>1.000</td></tr>
<tr><td>Reference</td><td>Ehlers et al. (2003)</td><td colspan="9">U.S. EPA (2004)</td><td>Li et al. (2019)</td><td>b</td></tr>
<tr><td>Fluorene</td><td>0.180</td><td colspan="9">0.890 [c]</td><td>0.248</td><td>1.000</td></tr>
<tr><td>Reference</td><td>Ehlers et al. (2003)</td><td colspan="9">U.S. EPA (2004)</td><td>Li et al. (2019)</td><td>b</td></tr>
<tr><td>2-Nitrobiphenyl</td><td colspan="10">1.000</td><td colspan="2">1.000</td></tr>
<tr><td>Reference</td><td colspan="10">b</td><td colspan="2">b</td></tr>
<tr><td>Phenanthrene</td><td>0.180</td><td colspan="9">0.890 [c]</td><td>0.301</td><td>1.000</td></tr>
<tr><td>Reference</td><td>Ehlers et al. (2003)</td><td colspan="9">U.S. EPA (2004)</td><td>Li et al. (2019)</td><td>b</td></tr>
<tr><td>Anthracene</td><td>0.180</td><td colspan="9">0.890 [c]</td><td>0.202</td><td>1.000</td></tr>
<tr><td>Reference</td><td>Ehlers et al. (2003)</td><td colspan="9">U.S. EPA (2004)</td><td>Li et al. (2019)</td><td>b</td></tr>
<tr><td>5-Nitroacenaphthene</td><td colspan="10">1.000</td><td colspan="2">1.000</td></tr>
<tr><td>Reference</td><td colspan="10">b</td><td colspan="2">b</td></tr>
<tr><td>Fluoranthene</td><td>0.180</td><td colspan="9">0.890 [c]</td><td>0.282</td><td>1.000</td></tr>
<tr><td>Reference</td><td>Ehlers et al. (2003)</td><td colspan="9">U.S. EPA (2004)</td><td>Li et al. (2019)</td><td>b</td></tr>
<tr><td>2-Nitrofluorene</td><td colspan="10">1.000</td><td colspan="2">1.000</td></tr>
<tr><td>Reference</td><td colspan="10">b</td><td colspan="2">b</td></tr>
</table>

Chemical species	*BAF* [a]											
	Ingestion										**Inhalation**	
	Soil	**Water**	**Vegetable**	**Fruit**	**Beef**	**Milk**	**Bird**	**Egg**	**Fish**	**Grain**	**Part. matter**	**Steam**
Pyrene	0.180	0.890 [c]	0.900 [d]								0.276	1.000
Reference	Ehlers et al. (2003)	U.S. EPA (2004)	Ramesh (2004)								Li et al. (2019)	[b]
9,10-Phenanthrenequinone	1.000										1.000	
Reference	[b]										[b]	
Retene	0.180	0.890 [c]									1.000	
Reference	Ehlers et al. (2003)	U.S. EPA (2004)									[b]	
9-Nitrophenanthrene	1.000										1.000	
Reference	[b]										[b]	
9-Nitroantracene	1.000										1.000	
Reference	[b]										[b]	
Benzo[*a*]fluorenone	1.000										1.000	
Reference	[b]										[b]	
Benzo[*a*]anthracene	0.180	0.890 [c]									0.055	1.000
Reference	Ehlers et al. (2003)	U.S. EPA (2004)									Li et al. (2019)	[b]
Chrysene	0.180	0.890 [c]									0.110	1.000
Reference	Ehlers et al. (2003)	U.S. EPA (2004)									Li et al. (2019)	[b]
1-Nitropyrene	1.000										1.000	
Reference	[b]										[b]	
Benzo[*b*]fluoranthene	0.180	0.890 [c]									0.061	1.000
Reference	Ehlers et al. (2003)	U.S. EPA (2004)									Li et al. (2019)	[b]
Benzo[*k*]fluoranthene	0.180	0.890 [c]									0.061	1.000
Reference	Ehlers et al. (2003)	U.S. EPA (2004)									Li et al. (2019)	[b]
Benzo[*e*]pyrene	0.180	0.890 [c]									1.000	
Reference	Ehlers et al. (2003)	U.S. EPA (2004)									[b]	
Benzo[*a*]pyrene	0.910	0.988 [c]									0.061	1.000
Reference	Ehlers et al. (2003)	Ramesh (2004)									Li et al. (2019)	[b]
6H-Benzo[*cd*]pyren-6-one	1.000										1.000	
Reference	[b]										[b]	

Chemical species	*BAF* [a]											
	Ingestion										**Inhalation**	
	Soil	**Water**	**Vegetable**	**Fruit**	**Beef**	**Milk**	**Bird**	**Egg**	**Fish**	**Grain**	**Part. matter**	**Steam**
Indeno[1,2,3-*cd*]pyrene	0.180	0.890 [c]									0.037	1.000
Reference	Ehlers et al. (2003)	U.S. EPA (2004)									Li et al. (2019)	[b]
6-Nitrobenzo[*a*]pyrene	1.000										1.000	
Reference	[b]										[b]	
Dibenzo[*a*,*h*]anthracene	0.180	0.890 [c]									0.067	1.000
Reference	Ehlers et al. (2003)	U.S. EPA (2004)									Li et al. (2019)	[b]
Benzo[*ghi*]perylene	0.180	0.890 [c]									0.043	1.000
Reference	Ehlers et al. (2003)	U.S. EPA (2004)									Li et al. (2019)	[b]
Pb	0.470 ± 0.067	0.110 ± 0.040 [d, f]	0.560 ± 0.255 [e]	0.450 ± 0.087 [e]	0.110 ± 0.040 [d, f]						0.145 ± 0.009	1.000
Reference	Hu et al. (2011)	NFESC (2000)	Hu et al. (2013)		NFESC (2000)						Julien et al. (2011)	[b]
Fe	0.039 ± 0.011	0.100	0.070	0.070	0.220	0.195 ± 0.173	0.350	0.350	0.350	0.900	1.000	
Reference	Hu et al. (2011)	Forth et al. (1973)	Ragan (1983)			Hallberg et al. (1992)	Fairweather-Tait et al. (1996)				[b]	
Zn	0.601 ± 0.086	0.400	0.680 ± 0.074 [e]	0.700 ± 0.108 [e]	0.500	0.300	0.500	0.500	0.500	0.150	0.755 ± 0.035	1.000
Reference	Hu et al. (2011)	EBRC (2007)	Hu et al. (2013)		Fairweather-Tait et al. (1996)						Julien et al. (2011)	[b]
Al	0.001	0.0028	0.003	0.003	0.001	0.001	0.001	0.001	0.003	0.001	1.000	
Reference	Hardisson et al. (2017)	Yokel et al. (2001)	Hardisson et al. (2017)								[b]	
Ba	1.000	0.070	0.180 [f]								0.193 ± 0.024	1.000
Reference	[b]	U.S. EPA (2004)	WHO (2001)								Julien et al. (2011)	[b]
Cu	0.298 ± 0.064	0.600	0.340 ± 0.084 [e]	0.370 ± 0.027 [e]	0.410	0.410	0.410	0.410	0.410	0.340	0.413 ± 0.041	1.000
Reference	Hu et al. (2011)	Weber et al. (1969)	Hu et al. (2013)		Lönnerdal (1996)						Julien et al. (2011)	[b]

Chemical species	*BAF* [a]											
	Ingestion										Inhalation	
	Soil	Water	Vegetable	Fruit	Beef	Milk	Bird	Egg	Fish	Grain	Part. matter	Steam
Cr(III)	0.058 ± 0.034	0.013	0.334 ± 0.144 [e]	0.600 ± 0.149 [e]	0.013 [d]						0.110 ± 0.040	1.000
Reference	Hu et al. (2011)	U.S. EPA (2004)	Hu et al. (2013)		U.S. EPA (2004)						Hu et al. (2012)	[b]
Cr(VI)	0.058 ± 0.034	0.025	0.334 ± 0.144 [e]	0.600 ± 0.149 [e]	0.100 [c]						0.110 ± 0.040	1.000
Reference	Hu et al. (2011)	U.S. EPA (2004)	Hu et al. (2013)		NFESC (2000)						Hu et al. (2012)	[b]
Se	1.000		0.550 ± 0.250 [d, f]								1.000	
Reference	[b]		U.S. EPA (2004)								[b]	
Ag	1.000	0.040	1.000								1.000	
Reference	[b]	U.S. EPA (2004)	[b]								[b]	
Sb	1.000	0.150	1.000								0.124 ± 0.019	1.000
Reference	[b]	U.S. EPA (2004)	[b]								Julien et al. (2011)	[b]
U	0.060										1.000	
Reference	Anke et al. (2009)										[b]	
Mn	0.476 ± 0.107	0.040	0.040 [d]								0.522 ± 0.034	1.000
Reference	Hu et al. (2011)	U.S. EPA (2004)									Julien et al. (2011)	[b]
Cd	0.745 ± 0.119	0.050	0.460 ± 0.039 [e]	0.450 ± 0.087 [e]	0.025 [d]						0.569 ± 0.038	1.000
Reference	Hu et al. (2011)	U.S. EPA (2004)	Hu et al. (2013)		U.S. EPA (2004)						Julien et al. (2011)	[b]
As	0.388 ± 0.057	0.950	0.950								0.457 ± 0.105	1.000
Reference	Hu et al. (2011)	U.S. EPA (2004)	National Research Council (1999)								Hu et al. (2012)	[b]
Co	0.221 ± 0.091	0.400									0.302 ± 0.032	1.000
Reference	Hu et al. (2011)	Leggett (2008)									Julien et al. (2011)	[b]

<table>
<tr><th rowspan="3">Chemical species</th><th colspan="12">BAF [a]</th></tr>
<tr><th colspan="10">Ingestion</th><th colspan="2">Inhalation</th></tr>
<tr><th>Soil</th><th>Water</th><th>Vegetable</th><th>Fruit</th><th>Beef</th><th>Milk</th><th>Bird</th><th>Egg</th><th>Fish</th><th>Grain</th><th>Part. matter</th><th>Steam</th></tr>
<tr><td>Hg</td><td>0.391 ± 0.148</td><td>0.070</td><td colspan="8">0.200 ± 0.050 [c, f]</td><td>1.000</td><td>0.770 ± 0.030 [f]</td></tr>
<tr><td>Reference</td><td>Hu et al. (2011)</td><td>U.S. EPA (2004)</td><td colspan="8">NFESC (2000)</td><td>[b]</td><td>U.S. EPA (2004)</td></tr>
<tr><td>Ni</td><td>0.157 ± 0.054</td><td>0.040</td><td>0.300 ± 0.033 [e]</td><td>0.320 ± 0.144 [e]</td><td colspan="6">0.040 [d]</td><td>0.292 ± 0.033</td><td>1.000</td></tr>
<tr><td>Reference</td><td>Hu et al. (2011)</td><td>U.S. EPA (2004)</td><td colspan="2">Hu et al. (2013)</td><td colspan="6">U.S. EPA (2004)</td><td>Julien et al. (2011)</td><td>[b]</td></tr>
<tr><td>V</td><td>0.112 ± 0.032</td><td colspan="9">0.010</td><td colspan="2">1.000</td></tr>
<tr><td>Reference</td><td>Hu et al. (2011)</td><td colspan="9">Treviño et al. (2019)</td><td colspan="2">[b]</td></tr>
<tr><td>Li</td><td colspan="10">1.000</td><td colspan="2">1.000</td></tr>
<tr><td>Reference</td><td colspan="10">[b]</td><td colspan="2">[b]</td></tr>
<tr><td>Br</td><td>1.000</td><td colspan="9">0.300</td><td colspan="2">1.000</td></tr>
<tr><td>Reference</td><td>[b]</td><td colspan="9">WHO (2005)</td><td colspan="2">[b]</td></tr>
<tr><td>Anthraquinone</td><td colspan="10">1.000</td><td colspan="2">1.000</td></tr>
<tr><td>Reference</td><td colspan="10">[b]</td><td colspan="2">[b]</td></tr>
<tr><td>6-Nitrochrysene</td><td colspan="10">1.000</td><td colspan="2">1.000</td></tr>
<tr><td>Reference</td><td colspan="10">[b]</td><td colspan="2">[b]</td></tr>
</table>

[a] Bioavailability factors for dermal contact with soil or water are already taken into account in the dose calculation (*ABS* and *PC*, respectively). Therefore, the *BAF* values must be 1.0;
[b] According to Health Canada (2004), *BAF* values of contaminants if ingested or inhaled should be considered as 1.0 when no specific values are found in literature;
[c] *BAF* value for general gastrointestinal absorption efficiency.
[d] *BAF* values for food;
[e] *BAF* obtained from the sum of the bioaccessible gastric fraction + bioaccessible intestinal fraction;
[f] Mean value of the *BAF* range found in the literature.

The uncertainty values not reported in the table correspond to 10% of the parameter value.

Table 14 – Chemical species carcinogenic classification

Chemical species	IARC (2019) Carcinogenic classification	U.S. EPA (2018)			
		Carcinogenic classification – Oral –	Oral mutagenic MOA	Carcinogenic classification – Inhalation –	Inhalation mutagenic MOA
p-Benzoquinone	3	n.a.	n.a.	n.a.	n.a.
Acetophenone	n.a.	D	-	n.a.	n.a.
Naphthalene	2B	C	-	n.a.	n.a.
1,4-Naphthoquinone	n.a.	n.a.	n.a.	n.a.	n.a.
Acenaphthylene	n.a.	D	-	D	-
Acenaphthene	3	D	-	D	-
Fluorene	3	D	-	D	-
2-Nitrobiphenyl	n.a.	n.a.	n.a.	n.a.	n.a.
Phenanthrene	3	D	-	D	-
Anthracene	3	D	-	D	-
5-Nitroacenaphthene	2B	n.a.	n.a.	n.a.	n.a.
Fluoranthene	3	D	-	D	-
2-Nitrofluorene	2B	n.a.	M-rpf	n.a.	M-rpf
Pyrene	3	D	-	D	-
9,10-Phenanthrenequinone	n.a.	n.a.	n.a.	n.a.	n.a.
Retene	n.a.	n.a.	n.a.	n.a.	n.a.
9-Nitrophenanthrene	3	n.a.	n.a.	n.a.	n.a.
9-Nitroantracene	3	n.a.	n.a.	n.a.	n.a.
Benzo[*a*]fluorenone	n.a.	n.a.	n.a.	n.a.	n.a.
Benzo[*a*]anthracene	2B	B2	M-rpf	B2	M-rpf
Chrysene	2B	B2	M-rpf	B2	M-rpf
1-Nitropyrene	2A	n.a.	M-rpf	n.a.	M-rpf
Benzo[*b*]fluoranthene	2B	B2	M-rpf	B2	M-rpf
Benzo[*k*]fluoranthene	2B	B2	M-rpf	B2	M-rpf
Benzo[*e*]pyrene	3	n.a.	n.a.	n.a.	n.a.
Benzo[*a*]pyrene	1	CH	M	CH	M
6H-Benzo[*cd*]pyren-6-one	n.a.	n.a.	n.a.	n.a.	n.a.
Indeno[1,2,3-*cd*]pyrene	2B	B2	M-rpf	B2	M-rpf
6-Nitrobenzo[*a*]pyrene	3	n.a.	n.a.	n.a.	n.a.
Dibenz[*a,h*]anthracene	2A	B2	M	B2	M
Benzo[*ghi*]perylene	3	D	-	D	-
Anthraquinone	2B	n.a.	n.a.	LH	-

Chemical species	IARC (2019) Carcinogenic classification	U.S. EPA (2018)			
		Carcinogenic classification – Oral –	Oral mutagenic action	Carcinogenic classification – Inhalation –	Inhalation mutagenic action
6-Nitrochrysene	2A	n.a.	M-rpf	n.a.	M-rpf
3-Nitrobenzanthrone	2B	n.a.	n.a.	n.a.	n.a.
Pb	2B	B2	-	B2	-
Fe	n.a.	n.a.	n.a.	n.a.	n.a.
Zn	n.a.	D	-	D	-
Al	n.a.	n.a.	n.a.	n.a.	n.a.
Ba	n.a.	InI	n.a.	NH	-
Cu	n.a.	D	-	D	-
Cr(III)	3	InI	n.a.	n.a.	n.a.
Cr(VI)	1	CH	-	D	-
Se	3	D	-	n.a.	n.a.
Ag	n.a.	D	-	D	n.a.
Sb	n.a.	n.a.	n.a.	n.a.	n.a.
U	n.a.	n.a.	n.a.	n.a.	n.a.
Mn	n.a.	D	-	n.a.	n.a.
Cd	1	B1	-	B1	-
As	1	A	-	A	-
Co	2B	n.a.	n.a.	n.a.	n.a.
Hg	3	D	-	D	-
Ni	1	A	-	n.a.	n.a.
V	n.a.	n.a.	n.a.	n.a.	n.a.
Li	n.a.	n.a.	n.a.	n.a.	n.a.
Br	n.a.	n.a.	n.a.	n.a.	n.a.

n.a. – No available; **-** – No mutagenic action; M - mutagenic and early life data lacking; M-rpf = relative potency factors were used to derive unit risk values based on the cancer risk of benzo[*a*]pyrene as the index chemical. In both cases, age-dependent adjustment factors should be applied when assessing risk for ages younger than 16 years.

IARC classification: **1** = carcinogenic; **2A** = probably carcinogenic; **2B** = possibly carcinogenic; **3** = not classifiable; **4** = probably not carcinogenic;

U.S. EPA (2005b) classification: **CH** = carcinogenic to humans; **LH** = likely to be carcinogenic; **SE** = suggestive evidence of carcinogenic potential;
InI = inadequate information to assess carcinogenic potential; **NH** = not likely to be carcinogenic

U.S. EPA (1986) classification: **A** = human carcinogen; **B1** = probable carcinogen, limited human evidence; **B2** = probable carcinogen, sufficient evidence in animals;
C = possible human carcinogen; **D** = not classifiable; **E** = evidence of non-carcinogenicity.

RADIOLOGICAL RISK

The implementation of the ***Radio_risk*** subroutine in HERisk allows to assess the radiological hazard associated with exposure to Naturally Occurring Radioactive Materials (NORM). Natural radiation sources constitute almost 80% of the collective radiation exposure of the world population. Pointedly, terrestrial background radiation due to natural radionuclides (^{238}U, ^{232}Th, ^{226}Ra and ^{40}K) represents the principal external source of radiation from the human body.

The radiological risk assessment implemented in HERisk is based on the methodologies established by the International Commission for Radiological Protection (ICRP, 1991), International Atomic Energy Agency (IAEA, 2003) and the United Nations Scientific Committee on the Effects of Atomic Radiation (UNSCEAR, 2000). The parameter values used in these calculations are summarized in **Table 16**.

Table 15 – Equations used by HERisk for radiological risk calculations

Description	Equation	Parameters used	Reference
Specific activity (Bq kg^{-1})	$A(t) = \frac{\ln 2 \cdot C_s(t) \cdot N_A}{MM \cdot t_{1/2}}$ (27)	***N_A*** = Avogadro´s number (atoms mol^{-1}); ***MM*** = Molar mass (mg mol^{-1}); ***$t_{1/2}$*** = Half-life time (s).	IAEA (2003)
Radium equivalent activity (Bq kg^{-1})	$Ra_{eq}(t) = A_U(t) + 1.43 \cdot A_{Th}(t) + 0.077 \cdot A_K(t)$ (28)	***A_U (t)*** = Specific activity for ^{238}U (Bq kg^{-1}); ***A_{Th} (t)*** = Specific activity for ^{232}Th (Bq kg^{-1}); ***A_K (t)*** = Specific activity for ^{40}K (Bq kg^{-1}). Permissible value: ≤ 370 Bq kg^{-1}	Belyaeva et al. (2019)
Absorbed dose rate (nGy h^{-1})	$AD(t) = 0.462 \cdot A_U(t) + 0.621 \cdot A_{Th}(t) + 0.0417 \cdot A_K(t)$ (29)		Belyaeva et al. (2019)
Indoor annual effective dose rate (mSv y^{-1})	$H_{eff}^{in}(t) = AD(t) \cdot DCF \cdot IF \cdot T_{exp}$ (30)	***AD (t)*** = Absorbed dose rate at time *t* (nGy h^{-1}); ***DCF*** = Dose conversion factor (mSv Gy^{-1}); ***IF*** – Indoor occupancy factor; ***T_{exp}*** = Exposure time (h y^{-1}). Permissible value: < 1 mSy	Belyaeva et al. (2019)
Outdoor annual effective dose rate (mSv y^{-1})	$H_{eff}^{out}(t) = AD(t) \cdot DCF \cdot OF \cdot T_{exp}$ (31)	***OF*** – Outdoor occupancy factor; Permissible value: < 1 mSy	Belyaeva et al. (2019)
Excess lifetime cancer risk due to indoor exposure	$ELCR_{in}(t) = \sum_{t=\Delta t}^{ED} H_{eff}^{in}(t) \cdot HLE \cdot RF$ (32)	***H_{eff}^{in} (t)*** = Indoor annual effective dose rate at time *t* (mSv y^{-1}); ***HLE*** = Human life expectancy (y); ***RF*** = Risk factor of contracting a fatal cancer per Sievert received (Sv^{-1}).	Belyaeva et al. (2019)

Description	Equation	Parameters used	Reference
Excess lifetime cancer risk due to outdoor exposure	$ELCR_{out}\ (t)\ = \sum_{t=\Delta t}^{ED} H_{eff}^{out}\ (t) \cdot HLE\ \cdot RF$ (33)	***H_{eff} ^{out} (t)*** = Outdoor annual effective dose rate at time *t* (mSv y^{-1}); ***HLE*** = Human life expectancy (y); ***RF*** = Risk factor of contracting a fatal cancer per Sievert received (Sv^{-1}).	Belyaeva et al. (2019)
Excess lifetime cancer risk due to indoor and outdoor exposure	$ELCR\ (t)\ = ELCR_{in}\ (t) + ELCR_{out}\ (t)$ (34)	***$ELCR_{in}$ (t)*** = Excess lifetime cancer risk due to indoor exposure; ***$ELCR_{out}$ (t)*** = Excess lifetime cancer risk due to outdoor exposure.	Belyaeva et al. (2019)
External hazard index	$H_{ex}\ (t)\ = 0.0027 \cdot\ A_U\ (t) + 0.00386 \cdot A_{Th}\ (t) + 0.0002 \cdot A_K\ (t)$ (35)	Permissible value: < 1 mSy	Agbalagba et al. (2012)
Internal hazard index	$H_{in}\ (t)\ = 0.0054 \cdot\ A_U\ (t) + 0.00386 \cdot A_{Th}\ (t) + 0.0002 \cdot A_K\ (t)$ (36)	Permissible value: < 1 mSy	Agbalagba et al. (2012)

Table 16 – Parameter values used for the radiological risk calculations

Parameter	Chemical species	Value	Reference
		Internal database	
MM (mg mol^{-1})	^{40}K	$3.99620 \cdot 10^{4}$	-
	^{226}Ra	$2.26030 \cdot 10^{5}$	
	^{232}Th	$2.32038 \cdot 10^{5}$	
	^{238}U	$2.38028 \cdot 10^{5}$	
$t_{1/2}$ (s)	^{40}K	$4.0366 \cdot 10^{16}$	-
	^{226}Ra	$5.1151 \cdot 10^{10}$	
	^{232}Th	$4.4340 \cdot 10^{17}$	
	^{238}U	$1.4160 \cdot 10^{17}$	
N_A (atoms mol^{-1})	-	$6.022 \cdot 10^{23}$	-
DCF (mSv Gy^{-1})	-	$0.7 \cdot 10^{-6}$	Belyaeva et al. (2019)
IF	-	0.8	Belyaeva et al. (2019)
OF	-	0.2	Belyaeva et al. (2019)
T_{exp} (h y^{-1})	-	8760	Belyaeva et al. (2019)
HLE (y)	-	78	U.S. EPA (2011)
RF (Sv^{-1})	-	0.05	Belyaeva et al. (2019)

ECOLOGICAL RISK

The ***Ecol_risk*** subroutine was implemented to assess the environmental pollution level and the possible toxic effects on organisms resulting from the chemical species concentration in various matrices (water, sediment and soil) of the studied areas. The ecological risk assessment methodology adopted in the HERisk is the result of a vast bibliographic review, which includes among other relevant works the followings: Jensen and Mesman (2006), Ogunkunle and Fatoba (2013), Pagliarini et al. (2019), Hakanson (1980) and Muller (1969). Among all indices reported, the 15 most used were included in the code. These indices are the most effective tools to evaluate the water, soil and sediment quality of a studied area by determining their respective level of contamination. Pollution indices were grouped into three different categories: single, combined and integrated. Some parameter values used in these calculations are summarized in **Table 18**, while the classifications of ecological risks are shown in **Table 19**.

Table 17 – Equations used by HERisk for ecological risk calculations

Description	Equation	Parameters used	Reference
	Single pollution indices		
Water, soil or sediment contamination factor	$CF_m\,(t) = \frac{C_m\,(t)}{C_{m\_ref}}$ (37)	$\boldsymbol{C_m\,(t)}$ = Chemical species concentration in the soil or sediment matrix at time t (mg kg^{-1}); $\boldsymbol{C_{m\_ref}}$ = Chemical species background concentration in the soil, sediment or water matrix (mg kg^{-1} or mg L^{-1});	Keshavarzi et al. (2019)
Water individual risk	$R_w\,(t) = 1 - \frac{1}{1 + CF_w\,(t)} = \frac{CF_w\,(t)}{1 + CF_w\,(t)}$ (38)	$\boldsymbol{CF_w\,(t)}$ = Water contamination factor at time t.	Pagliarini et al. (2019)
Geoaccumulation index	$I_{geo}^{m}\,(t) = log_2\left[\frac{C_m\,(t)}{1.5\cdot C_{m\_ref}}\right]$ (39)	$\boldsymbol{C_{m\_ref}}$ = Chemical species background concentration in the soil or sediment matrix (mg kg^{-1}).	Müller (1969)
Enrichment factor	$EF_m\,(t) = \frac{(C_m\,(t)/C_{m\_ref})}{(C_x\,(t)/C_{x\_ref})}$ (40)	$\boldsymbol{C_{m\_ref}}$ = Chemical species background concentration in the soil or sediment matrix (mg kg^{-1}); $\boldsymbol{C_x\,(t)}$ = Reference chemical species concentration (Al, Fe or Mn) in the soil or sediment matrix at time t (mg kg^{-1}); $\boldsymbol{C_{x\_ref}}$ = Reference chemical species background concentration in the sediment matrix (mg kg^{-1}) or for soil matrix was used the reference chemical species concentration in the upper continental crust ($\boldsymbol{C_{UCC}}$) (mg kg^{-1}).	Emenike et al. (2020)
Single pollution index	$PI_m\,(t) = \frac{C_m\,(t)}{C_{UCC}}$ (41)	$\boldsymbol{C_{UCC}}$ = Chemical species concentration in the upper continental crust (mg kg^{-1}).	Emenike et al. (2020)

Combined pollution indices			
Pollution load index	$$PLI_m(t) = \sqrt[n]{\prod_{j=1}^{n} CF_m^j(t)} \quad (42)$$	$\boldsymbol{CF_{m,i}(t)}$ = Matrix contamination factor due to chemical species *j* at time *t*; ***n*** = Number of chemical species.	Doležalová Weissmannová et al. (2019)
Water combined risk	$$R_{W-comb}(t) = 1 - \left[\prod_{j=1}^{n} (1 - R_w(t))_j\right] \quad (43)$$	$\boldsymbol{R_{Wi}(t)}$= Water individual risk for chemical species *j* at time *t*.	Pagliarini et al. (2019)
Modified degree of contamination	$$mC_d(t) = \sum_{j=1}^{n} CF_{m,j}(t) \quad (44)$$		Hakanson (1980)
Integrated threshold pollution index	$$IPI_{Th}(t) = \frac{1}{n} \cdot \sum_{j=1}^{n} \left(\frac{C_m(t)}{C_{TL}}\right)_j \quad (45)$$	$\boldsymbol{C_{TL}}$ = Guideline value established by the national legislation for the chemical specie *j* (mg kg^{-1} or mg L^{-1}).	Qingjie et al. (2008)
Potential ecological risk index	$$PERI_m(t) = \sum_{j=1}^{n} T_r^j \cdot CF_m^j(t) \quad (46)$$	$\boldsymbol{T_r}$ – Toxic response factor of the chemical specie *j*.	Emenike et al. (2020)
Nemerov pollution index	$$PI_{Nem}(t) = \sqrt{\frac{\langle PI_m(t)\rangle^2 + (PI_m^{max}(t))^2}{2}} \quad (S30)$$	$\boldsymbol{\langle PI_m(t)\rangle}$ = Average values of the single pollution index at time *t*; $\boldsymbol{PI_m^{max}(t)}$ = Maximum obtained value of the single pollution index at time *t*.	Keshavarzi et al. (2019)
Mean probable effect level quotient	$$m-PEL-q(t) = \frac{1}{n} \cdot \sum_{j=1}^{n} \left(\frac{C_m(t)}{PEL}\right)_j \quad (S31)$$	***PEL*** = Probable effect level (mg kg^{-1}).	Fairey et al. (2001)
Mean effects range-median quotient	$$m-ERM-q(t) = \frac{1}{n} \cdot \sum_{j=1}^{n} \left(\frac{C_m(t)}{ERM}\right)_j \quad (S32)$$	***ERM*** = Effects range-median (mg kg^{-1}).	Fairey et al. (2001)
Toxic risk index	$$TRI(t) = \sum_{j=1}^{z} \sqrt{\frac{\left(\frac{C_m(t)}{PEL}\right)_j^2 + \left(\frac{C_m(t)}{TEL}\right)_j^2}{2}} \quad (S33)$$	***TEL*** = Threshold effect limit (mg kg^{-1}).	Emenike et al. (2020)
Integrated pollution indices			
Mean distribution coefficient Log	$$K_{d\_MPI}(t) = log\left[\frac{PLI_{sed}(t)}{MPI(t)}\right] \quad (S34)$$	$\boldsymbol{PLI_{sed}(t)}$ = Sediment pollution load index at time *t*; $\boldsymbol{MPI(t)}$ = Metal pollution index at time *t*.	Sedeño-Díaz et al. (2019)

Integrated pollution indices			
	Chemical Line of Evidence		
Toxic pressure	$TP_j\ (t) = \dfrac{1}{1 + e^{-\left(\frac{\log(C_m)-\alpha}{\beta}\right)_j}} \quad (S35)$	$\boldsymbol{\alpha}$ = log-transformed value of the toxicity of the chemical species *j*; $\boldsymbol{\beta}$ = Slope parameter of the Specie Sensitivity Distribution for chemical species *j* toxicity data.	Son et al. (2019)
Background toxic pressure	$TP_{BG,j}\ (t) = \dfrac{1}{1 + e^{-\left(\frac{\log(C_{m\_ref})-\alpha}{\beta}\right)_j}} \quad (S36)$		Son et al. (2019)
Corrected toxic pressure	$TP_j{}'\ (t) = \dfrac{TP_j\ (t) - TP_{BG,j}\ (t)}{1 - TP_{BG,j}\ (t)} \quad (S37)$	$\boldsymbol{TP_j\ (t)}$ = Toxic pressure of chemical species *j* at time *t*; $\boldsymbol{TP_{BG,j}\ (t)}$ = Background toxic pressure of chemical species *j* at time *t*.	Son et al. (2019)
Risk value for Chemical Line of Evidence	$Risk_{ChemLoE}\ (t) = 1 - \left[\prod_{j=1}^{n} \left(1 - TP_j{}'\ (t)\right)_j\right] \quad (S38)$	$\boldsymbol{TP_j{}'\ (t)}$ = Corrected toxic pressure of chemical species *j* at time *t*.	Son et al. (2019)
Integrated risk for Chemical Line of Evidence	$IR_{ChemLoE}\ (t) = 1 - (10^{\Gamma}) \qquad \Gamma = \dfrac{1}{m}\sum_{k=1}^{m} \log(1 - Risk_{ChemLoE}\ (t))_k \quad (10)$	$\boldsymbol{Risk_{ChemLoE}}$ = Risk value for Chemical Line of Evidence for environmental compartment *m*; $\boldsymbol{m}$ = Number of environmental compartments.	Son et al. (2019)

Table 18 – Some parameter values used for the ecological risk calculations

Chemical species	C_{soil_ref} [a] (mg kg^{-1})	C_{TL_soil} [b] (mg kg^{-1})	C_{water_ref} and C_{TL_water} [c] (mg L^{-1})	C_{UCC} [d] (mg kg^{-1})	T_r [*]	α [**]	β [**]
Cu	5.94	200.00	9.00E-3	28.00	5.00	2.78	0.3914
Zn	45.41	450.00	1.80E-1	67.00	1.00	3.32	0.3970
Mn	173.41	n.d.	1.00E-1	774.6	1.00	n.d.	n.d.
Ni	7.63	70.00	2.50E-2	47.00	5.00	2.81	0.4355
Pb	19.48	180.00	1.00E-2	17.00	5.00	3.69	0.4852
Co	3.50	35.00	5.00E-2	17.30	5.00	3.23	0.6120
Fe	16048.09	n.d.	3.00E-1	39000.00	n.d.	n.d.	n.d.

n.d. - not determined; [a] Values taken from Biondi et al. (2011) and da Silva et al. (2015); [b] Values taken from CONAMA (2009); [c] Values taken from CONAMA (2005); [d] Values taken from Rudnick et al. (2014); [*] Values taken from Hakanson (1980) and Ullah et al. (2019); [**] Values taken from Rutgers et al. (2008).

Table 19 – Ecological risks characterizations

Category	**0**	**1**	**2**	**3**	**4**	**5**	**6**
Contamination level	Unpolluted	Low to moderately polluted	Moderately polluted	Moderately to heavily polluted	Heavily polluted	Heavily to extremely polluted	Extremely polluted
CF_m	< 1	–	1 – 3	–	3 – 6	–	≥ 6
$R_{w\text{-}comb}$	–	≤ 0.25	0.25 – 0.50	–	0.50 – 0.75	–	≥ 0.75
mC_d	< 1.5	1.5 – 2.0	2.0 – 4.0	4.0 – 8.0	8.0 – 16.0	16.0 – 32.0	≥ 32
IPI_{Th}	–	≤ 1	1 – 3	–	–	–	≥ 3
EFact	< 1	1 – 3	3 – 5	5 – 10	10 – 25	25 – 50	≥ 50
I_{geo}	≤ 0	0 – 1	1 – 2	2 – 3	3 – 4	4 – 5	≥ 5
PI_{Nem}	< 0.7	0.7 – 1	1 – 2	2 – 3	≥ 3	–	–

Category	**0**	**1**	**2**	**3**	**4**	**5**
Risk	Negligible	Low	Moderate	Considerable	High	Extreme
PERI	–	< 150	150 – 300	–	300 – 600	≥ 600
m–PEL–q	–	≤ 0.1	0.1 – 1	–	≥ 1	–
TRI	≤ 5	5 – 10	10 – 15	15 – 20	≥ 20	–
$IR_{ChemLoE}$	≤ 0.20	–	0.20 – 0.75	–	≥ 0.75	–

Category	**1**	**2**	**3**	**4**
Probability of being toxic	9 %	21%	49%	76%
m–ERM–q	< 0.1	0.11 – 0.50	0.51 – 1.50	≥ 1.50

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