RISK-NET

USER GUIDE

Version 3.2
May 2024

RECONnet
Italian Network on the Management and
Remediation of Contaminated Sites

RISK-NET

TOOL FOR THE RISK ASSESSMENT OF CONTAMINATED SITES

The **Risk-net** software was designed to perform the calculations required for the Risk-Based Corrective Action (RBCA) planning process, as defined in the Italian national guidelines for risk assessment that are based on the ASTM E-2081-00 Standard Guide for Risk-Based Corrective Action and ASTM E-1739-95 Standard Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites.

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Credits
This version of the software has been developed based on the Risk-net 3.0 version (2018) created by Iason Verginelli (University of Rome Tor Vergata) and Alessandro Girelli (I.A. Industria Ambiente S.r.l.).

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Risk-net can be downloaded for free from the website of the ***Reconnet*** *network at* www.reconnet.net

Ref: Verginelli I. (2024). Risk-net User Guide. Version 3.2. Rome, Italy, Reconnet.

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DESCRIPTION OF THE SOFTWARE

The Risk-net software has been developed within the Reconnet network with the aim of providing a tool based on the Italian ISPRA guidelines for risk analysis application, developed following the ASTM RBCA (Risk-Based Corrective Action) standard approach. The software allows to apply the risk assessment procedure both in forward and backward mode, thus evaluating the risk or the clean-up objective for a contaminated site, respectively.

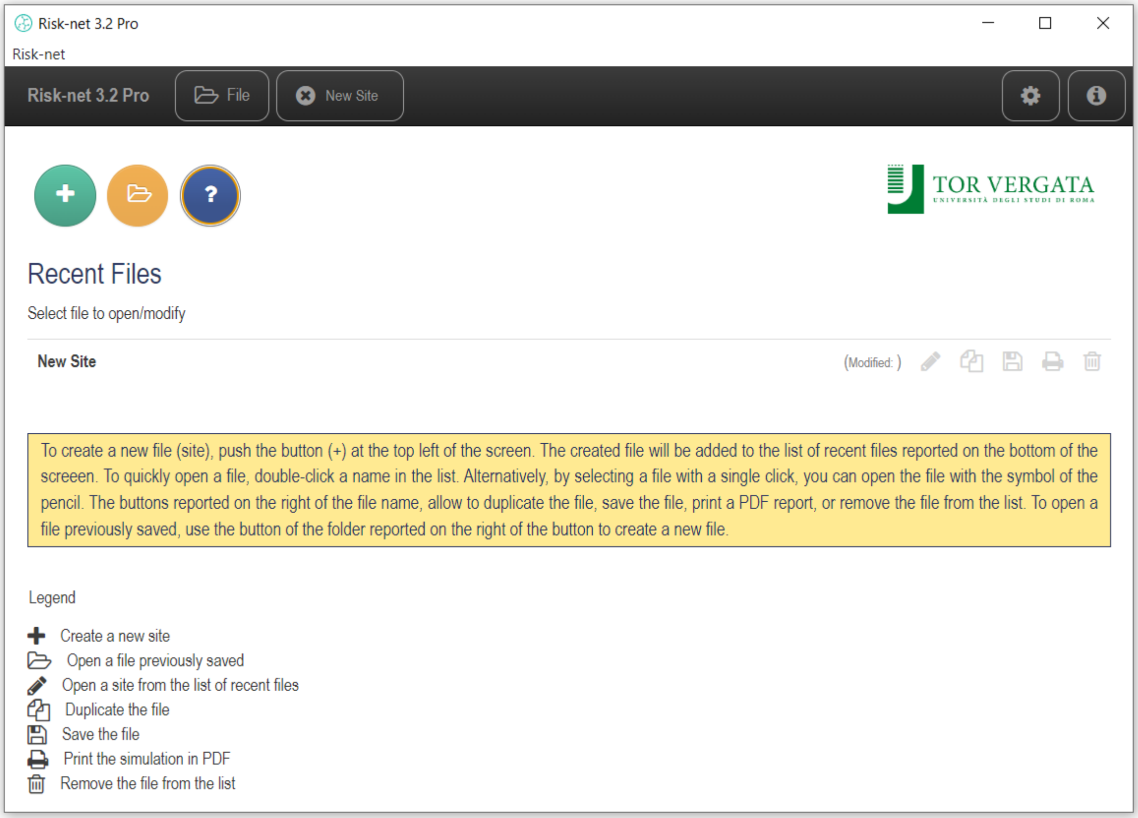
Namely for each exposure pathway activated by the user, Risk-net calculates, through the Fate and Transport (F&T) models described in the ISPRA guidelines (2008), the maximum steady state concentrations expected at the point of exposure. Next, based on the exposure parameters defined by the user, the daily dose assumed by each receptor considered is calculated. These doses combined with the corresponding toxicological parameters are used for the calculation of risk and remediation targets (SSTL, Site-Specific Target Levels) for each contaminant and active route. Finally, the effects related to the presence of multiple routes of exposure and multi-component contamination is calculated.

The key features of Risk-net include:

- *Risk-Based Cleanup Level Calculations:* Risk-net completes all calculations required for Tier 1 and Tier 2 RBCA evaluations, including: risk-based exposure limits and attenuation factor derived from simple fate and transport models.
- *Fate and Transport Models:* Validated analytical models for air, groundwater and soil exposure pathways, including all models used in the ISPRA (2008) standard.
- *Chemical and Toxicological Database:* Integrated toxicological and chemical parameter library preloaded (ISS-INAIL Database). The database is customizable by the user, including import features for management of external database.
- *User-Friendly Interface:* Point-and-click graphical user interface with on-line help, unit conversion and Load/Save capability.

MAIN SCREEN

The main screen is automatically opened at startup (Figure 1). On this screen it is possible to create a new simulation file and manage the simulation files previously created. To create a new file (site), push the button (+) at the top left of the screen. The created file will be added to the list of recent files reported on the bottom of the screen. To quickly open a file, double-click a name in the list. Alternatively, by selecting a file with a single click, the user can open the file with the symbol of the pencil. The buttons reported on the right of the file name, allow to duplicate the file, save the file, print a PDF report, or remove the file from the list. To open a file previously saved, use the button of the folder reported on the right of the button to create a new file. Table 1 reports a brief description of the symbols present in the main screen.



To create a new file (site), push the button (+) at the top left of the screen. The created file will be added to the list of recent files reported on the bottom of the screeen. To quickly open a file, double-click a name in the list. Alternatively, by selecting a file with a single click, you can open the file with the symbol of the pencil. The buttons reported on the right of the file name, allow to duplicate the file, save the file, print a PDF report, or remove the file from the list. To open a file previously saved, use the button of the folder reported on the right of the button to create a new file.

Legend

- ✚ Create a new site
- 📂 Open a file previously saved
- ✎ Open a site from the list of recent files
- ⧉ Duplicate the file
- 💾 Save the file
- 🖶 Print the simulation in PDF
- 🗑 Remove the file from the list

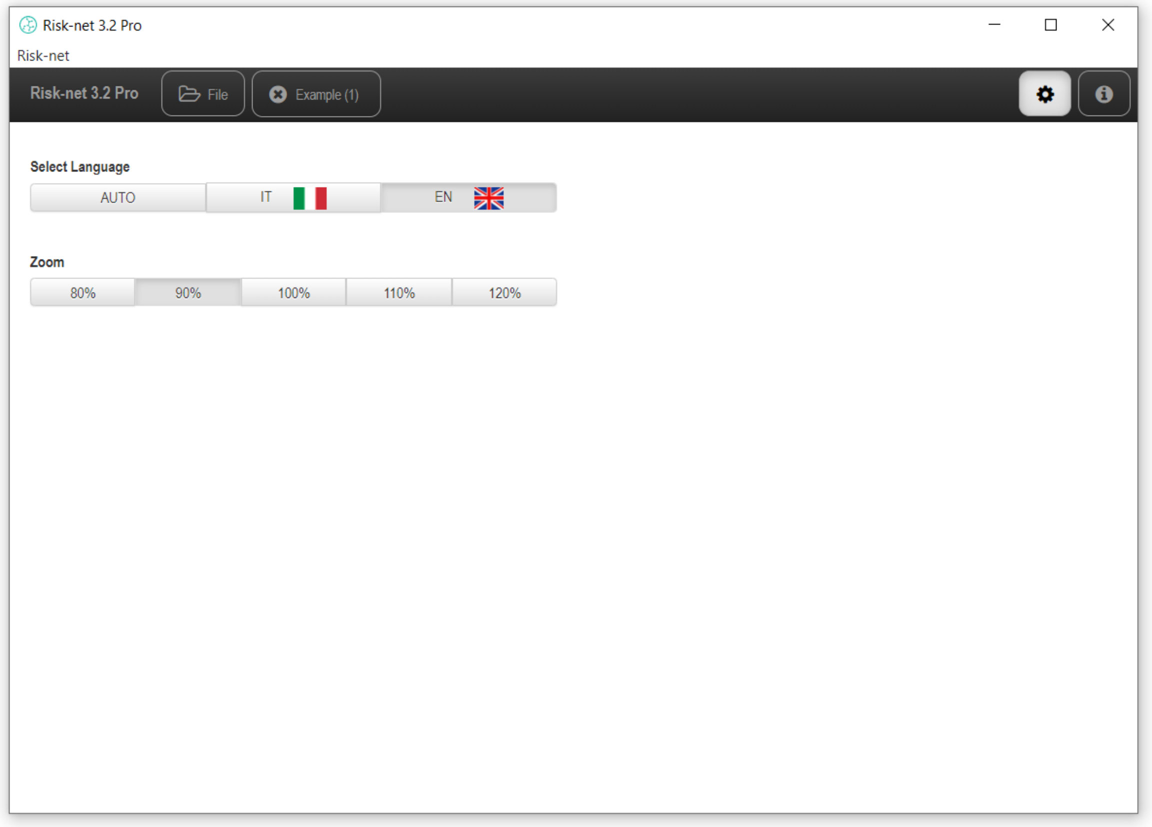
Figure 1. Main screen of the software Risk-net.

Please note that the software automatically saves up to 5 files internally to the software. This option prevents data loss in the event of accidental closure of the program. This automatic saving is applied to the 5 most recent files and therefore it is suggested to save locally the files with the dedicated button at the end of each simulation.

Table 1. Description of the symbols present in the main screen.

Button	Function
+	**Create a new site**
📂	**Open a file previously saved**
?	**Help**
✎	**Open a site from the list of recent files**
⧉	**Duplicate the file**
💾	**Save the file**
🖨	**Print the simulation in PDF**
🗑	**Remove the file from the list**
⚙	**Settings**

To change the language or the zoom of the windows, from the main screen by clicking on the “Settings” button, the user can access the screen shown in Figure 2. To return to the main screen, simply click on the "File" button at the top left.



Select Language

AUTO | IT | EN

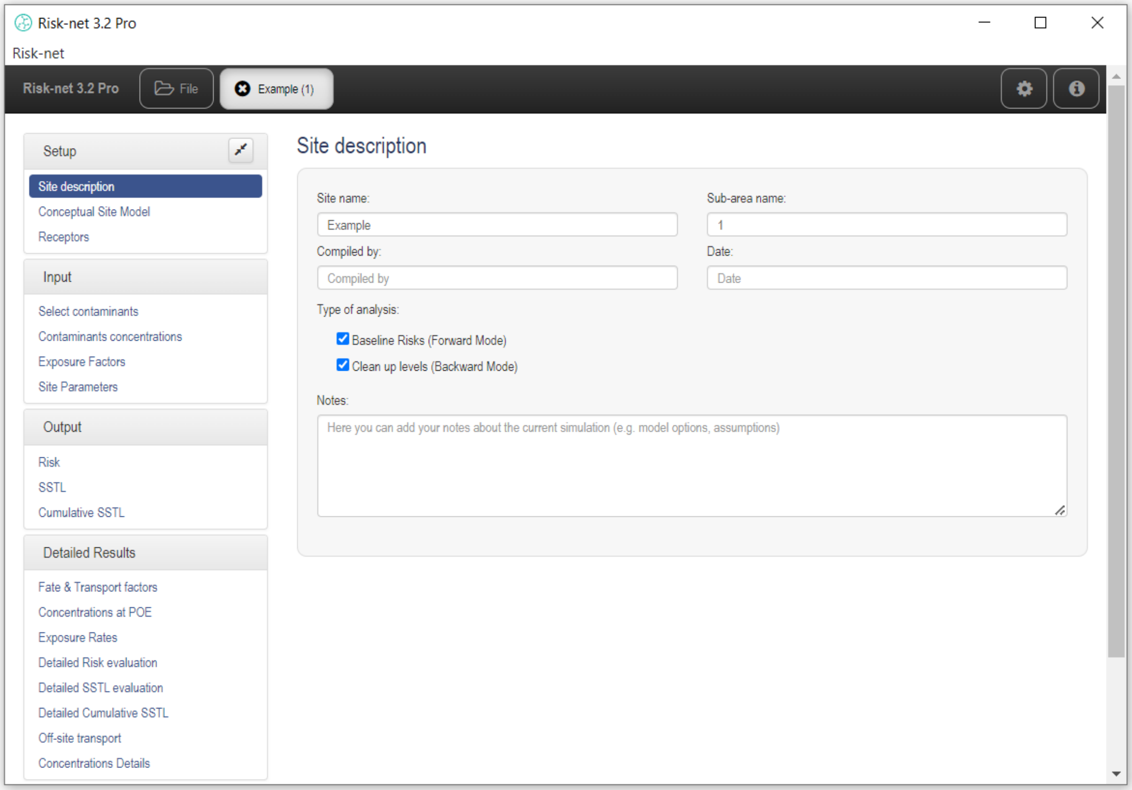
Zoom

80% | 90% | 100% | 110% | 120%

Figure 2. Main Settings.

SIMULATION SCREEN

When opening a new file, the user accesses the screen shown in Figure 3. On this screen, using the lateral menu, the user can quickly access the various input and output screens. If the software is used on computers with small screens, the side menu can be deactivated using the button in the upper right part of the menu. In this case, the menu for accessing the various input and output screens is positioned horizontally as shown in Figure 4.

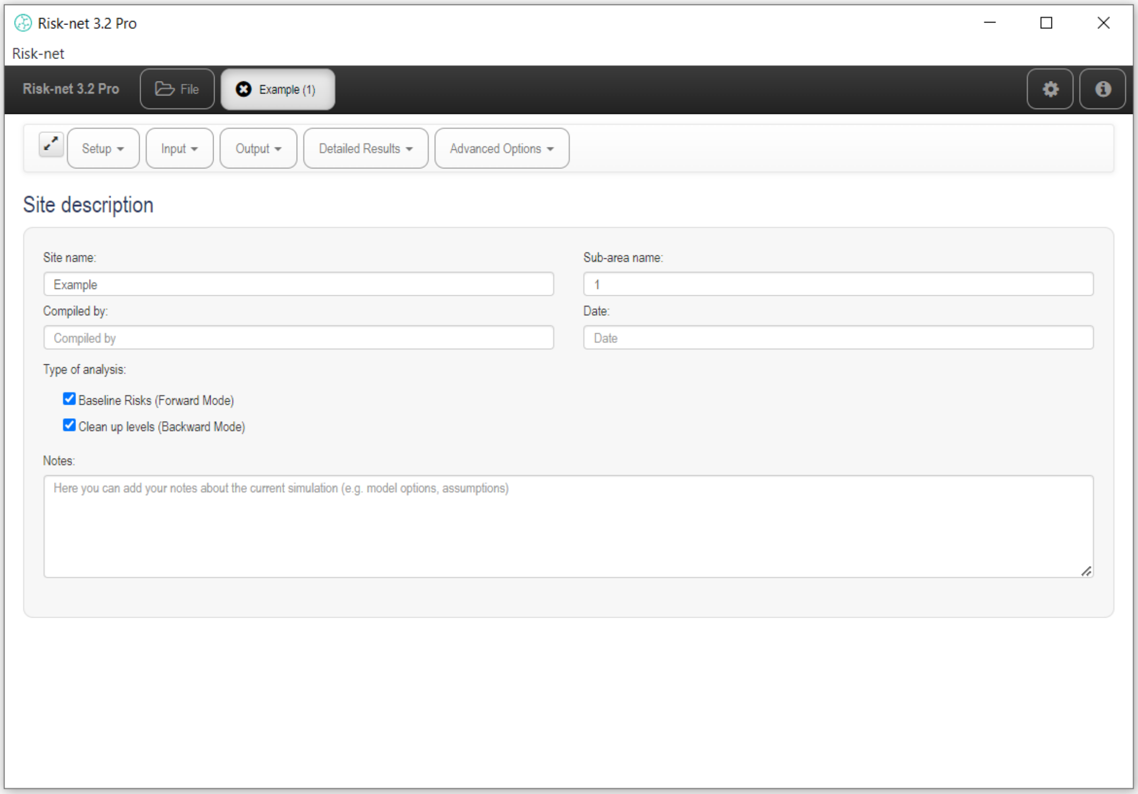


Site description

Site name: Example
Sub-area name: 1
Compiled by: Compiled by
Date: Date
Type of analysis:
☑ Baseline Risks (Forward Mode)
☑ Clean up levels (Backward Mode)
Notes: Here you can add your notes about the current simulation (e.g. model options, assumptions)

Figure 3. Simulation screen with activated lateral menu.

To reset the lateral menu just press the button .



Site description

Site name: Example

Sub-area name: 1

Compiled by: Compiled by

Date: Date

Type of analysis:

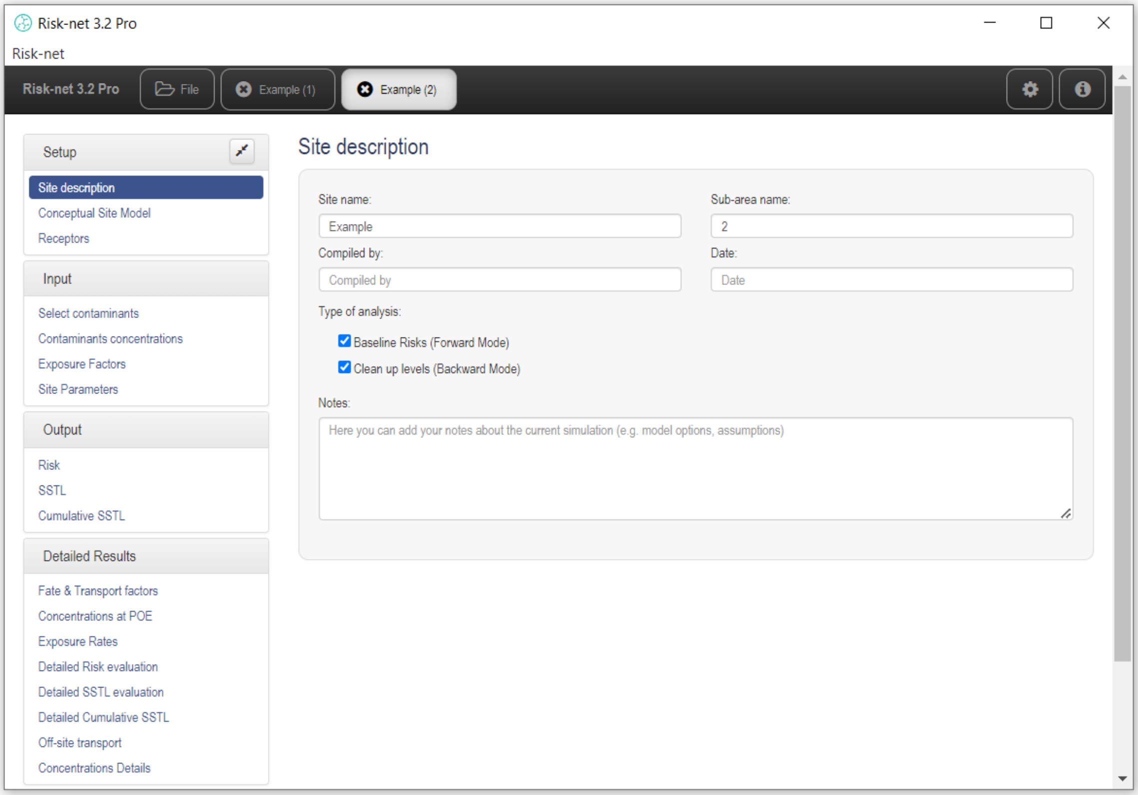
☑ Baseline Risks (Forward Mode)

☑ Clean up levels (Backward Mode)

Notes: Here you can add your notes about the current simulation (e.g. model options, assumptions)

Figure 4. Simulation screen without lateral menu.

The software allows the user to open multiple simulation files as shown in Figure 5. In this case it is possible to move from one simulation file to the other by clicking on the name of the tab at the top of the screen. To close a simulation file, simply press the button ✖ that appears to the right of the file name. Note that the simulation file is automatically saved in the recent files list and therefore closing the simulation file does not result in data loss. To save the file locally on computer the user must go back to the main screen through the "File" button on the top left of the software screen and follow the instructions described in the previous section.



Site description

Site name: Example

Sub-area name: 2

Compiled by: Compiled by

Date: Date

Type of analysis:

☑ Baseline Risks (Forward Mode)

☑ Clean up levels (Backward Mode)

Notes:

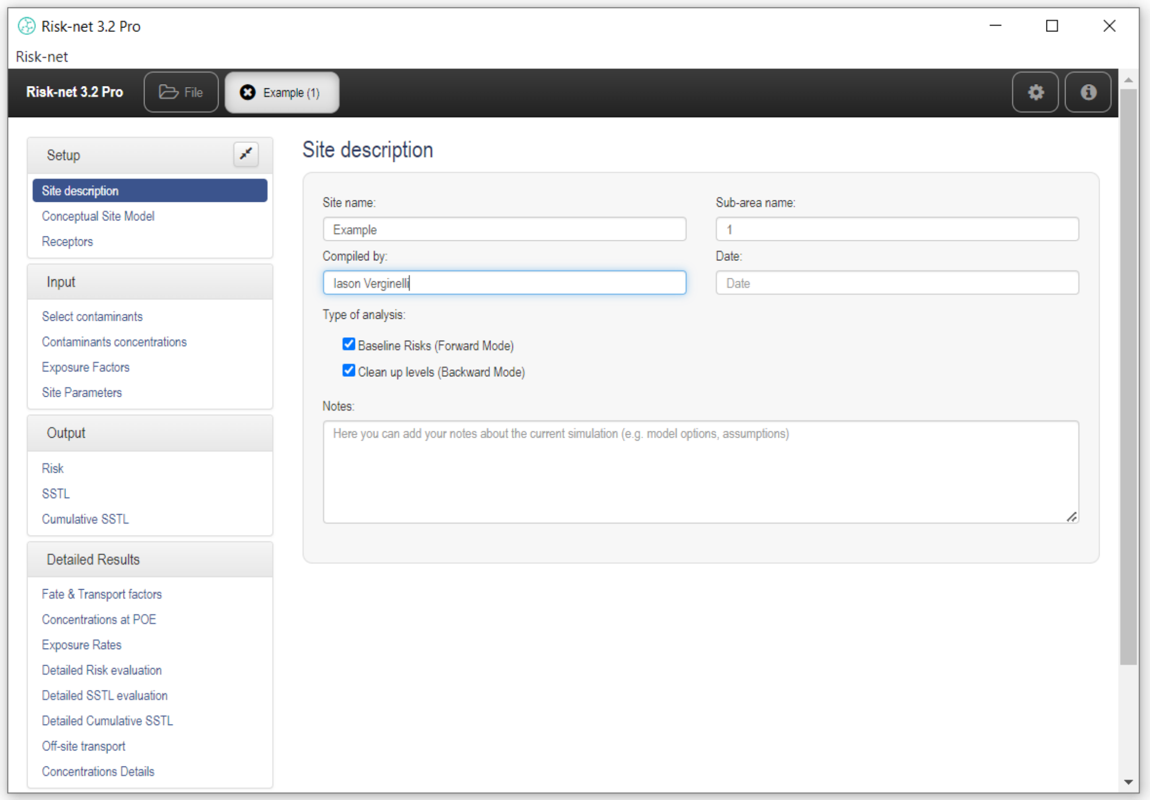
Here you can add your notes about the current simulation (e.g. model options, assumptions)

Figure 5. Multiple files open.

SIMULATION SETUP

SITE DESCRIPTION

This screen (Figure 6) is accessed by clicking "Site description" on the "Setup" menu.



Site description

Site name: Example

Sub-area name: 1

Compiled by: Iason Verginelli

Date: Date

Type of analysis:

☑ Baseline Risks (Forward Mode)

☑ Clean up levels (Backward Mode)

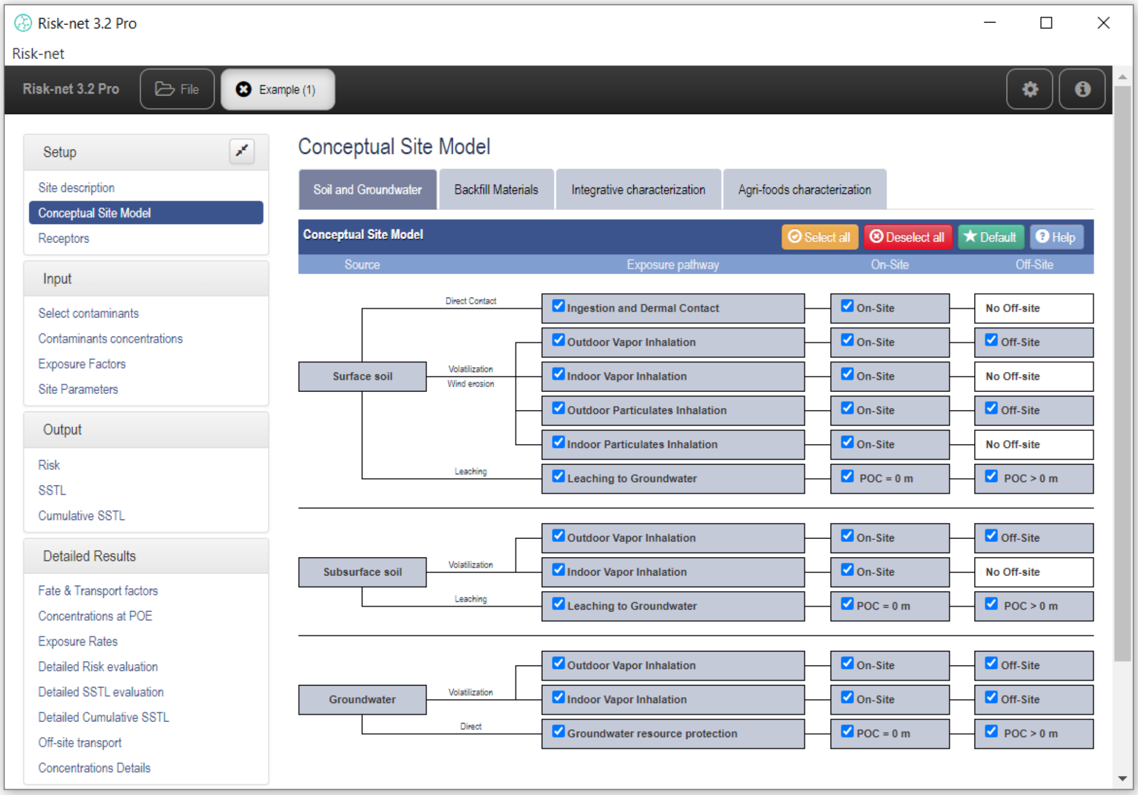
Notes: Here you can add your notes about the current simulation (e.g. model options, assumptions)

Figure 6. Site description.

On this screen it is possible to define the general information of the project (Name of the site, name of the eventual sub-area, Date, and Compiled By). It should be noted that in the list of temporary files the name of the simulation will be automatically set based on the "Name of the site" and the name of the sub-area (in brackets) assigned on this screen. The "Notes" box allows the user to add some notes on the compilation of the project. On this screen it is also possible to select the type of analysis to be performed. In particular, the user can decide whether to perform only a forward analysis for the calculation of the risks, only the backward mode for the calculation of the clean-up levels or both. In the event that one of the two types of analysis is deactivated (backward or forward mode) the Risks and/or SSTL screens are not shown.

CONCEPTUAL SITE MODEL

This screen (Figure 7) is accessed by clicking "Conceptual Site Model" on the "Setup" menu.



Source		Exposure pathway	On-Site	Off-Site
Surface soil	Direct Contact	☑ Ingestion and Dermal Contact	☑ On-Site	No Off-site
	Volatilization Wind erosion	☑ Outdoor Vapor Inhalation	☑ On-Site	☑ Off-Site
		☑ Indoor Vapor Inhalation	☑ On-Site	No Off-site
		☑ Outdoor Particulates Inhalation	☑ On-Site	☑ Off-Site
		☑ Indoor Particulates Inhalation	☑ On-Site	No Off-site
	Leaching	☑ Leaching to Groundwater	☑ POC = 0 m	☑ POC > 0 m
Subsurface soil	Volatilization	☑ Outdoor Vapor Inhalation	☑ On-Site	☑ Off-Site
		☑ Indoor Vapor Inhalation	☑ On-Site	No Off-site
	Leaching	☑ Leaching to Groundwater	☑ POC = 0 m	☑ POC > 0 m
Groundwater	Volatilization	☑ Outdoor Vapor Inhalation	☑ On-Site	☑ Off-Site
		☑ Indoor Vapor Inhalation	☑ On-Site	☑ Off-Site
	Direct	☑ Groundwater resource protection	☑ POC = 0 m	☑ POC > 0 m

Figure 7. Conceptual Site Model.

On this screen the user must define the exposure scenario by selecting the contaminated media(s), fate and transport pathways (if any), and associated exposure routes. Namely, the user needs to identify those pathways that are likely to be complete, based on knowledge of the locations of impacted soil or groundwater relative to the location and habits of people that might be exposed to the chemicals of concern.

The risks and the SSTLs can be calculated for the following secondary sources: surface soil (0-1 m from ground level), subsurface soil (>1m) and groundwater. For each matrix the user must activate the exposure/migration pathway and then activate the type of receptor (on-site, off-site or both).

In Risk-net the following exposure pathways can be activated:

<u>Surface Soil</u>

- Dermal contact

- Soil ingestion
- Outdoor vapor inhalation
- Indoor vapor inhalation
- Outdoor particulate inhalation
- Indoor particulate inhalation
- Leaching to groundwater

Subsurface Soil

- Outdoor vapor inhalation
- Indoor vapor inhalation
- Leaching to groundwater

Groundwater

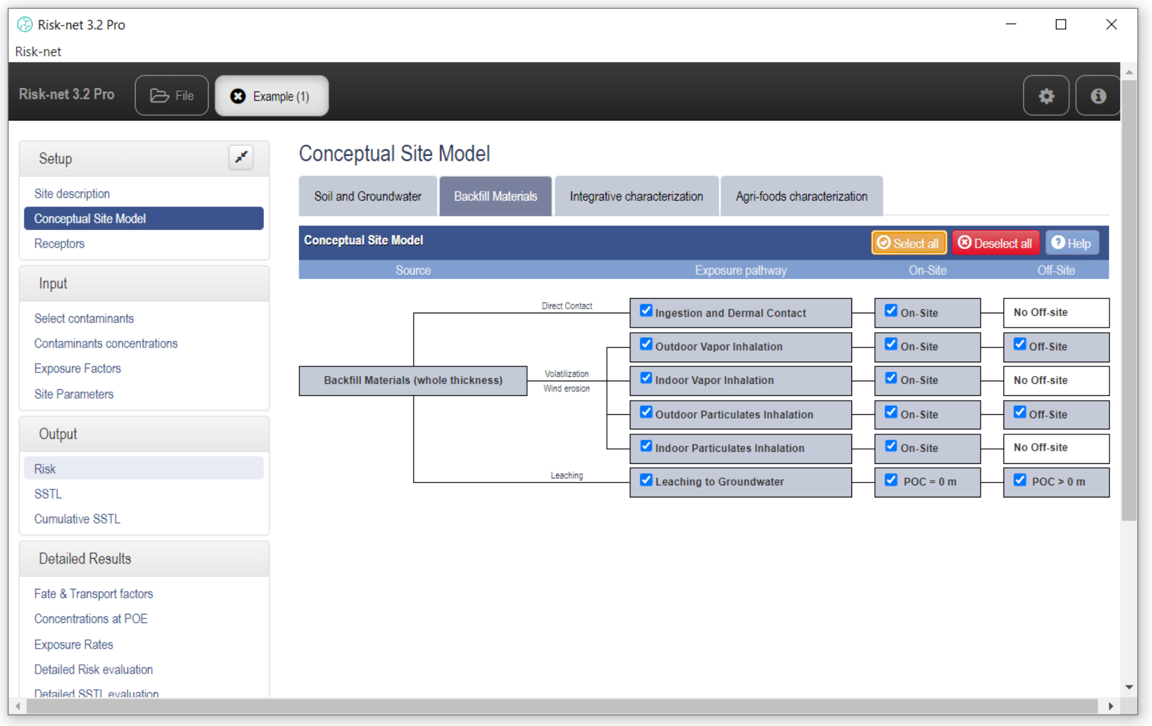
- Outdoor vapor inhalation
- Indoor vapor inhalation
- Groundwater resource protection

In this context, the term “on-site” refers to a receptor located above the source zone, whereas “off-site” refers to a receptor at any point away from the source zone.

The different check boxes of the exposure pathways and the associated receptors are highlighted in blue if activated. If no target is activated for an activated exposure pathway, this is highlighted in red indicating an incomplete reconstruction of the conceptual site model.

As to the leaching and protection of the groundwater resource, the terms POC reported on the screen refer to the point of compliance. Thus, if the box "POC = 0 m" is activated, the risk for the groundwater resource (if activated in the Receptors screen) in the case of leaching from surface and subsurface soil is calculated by comparing the expected concentrations in groundwater below the source zone (i.e. no attenuation due to groundwater transport and dispersion) and the limit values defined by the groundwater legislation (e.g. MCL, maximum contaminant level). It is worth noting that although the software allows to activate both options (i.e. POC = 0 m and POC> 0 m) it is evident that if both are activated, the final SSTLs calculated for the protection of the groundwater resource will be those estimated considering POC = 0 m. Therefore, the user must pay particular attention to which of the two options keep activated.

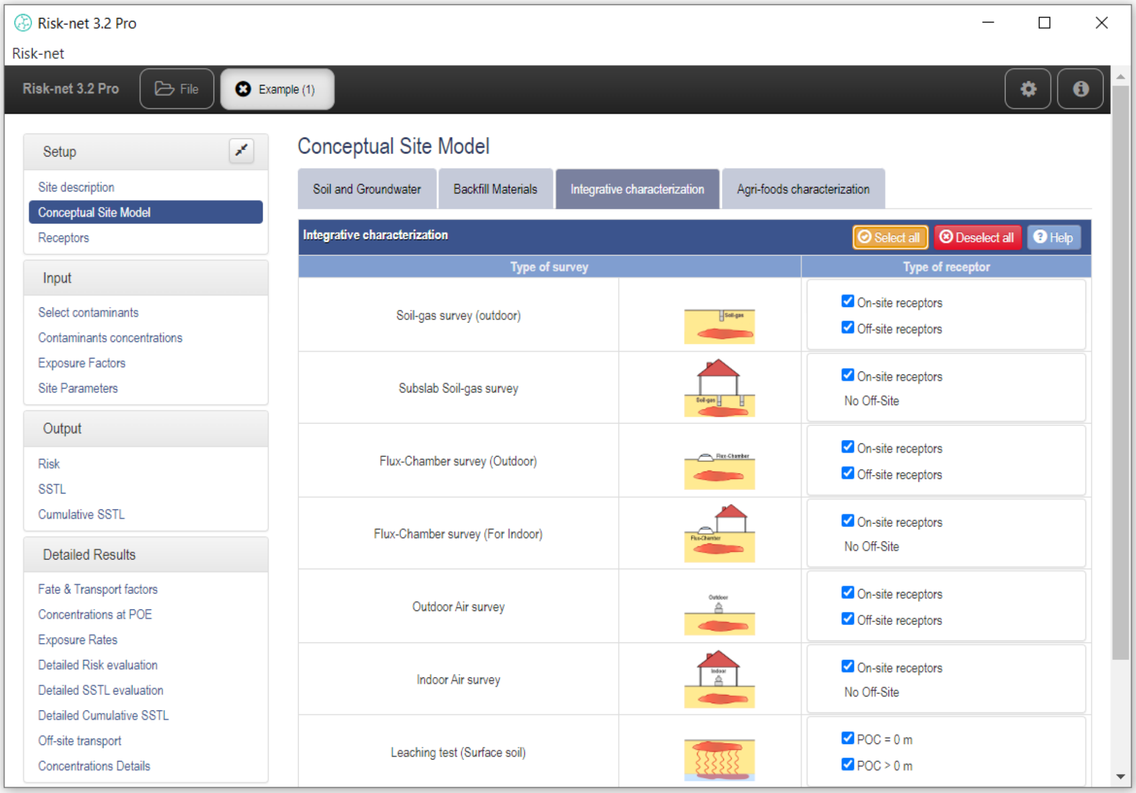
By clicking on the “Backfill Materials” tab the user accesses the screen shown in Figure 8. In this screen it is possible to select the migration and exposure routes active on the site for the Backfill Materials.



☑ Ingestion and Dermal Contact — ☑ On-Site — No Off-site
☑ Outdoor Vapor Inhalation — ☑ On-Site — ☑ Off-Site
☑ Indoor Vapor Inhalation — ☑ On-Site — No Off-site
☑ Outdoor Particulates Inhalation — ☑ On-Site — ☑ Off-Site
☑ Indoor Particulates Inhalation — ☑ On-Site — No Off-site
☑ Leaching to Groundwater — ☑ POC = 0 m — ☑ POC > 0 m

Figure 8. Conceptual model for Backfill Materials.

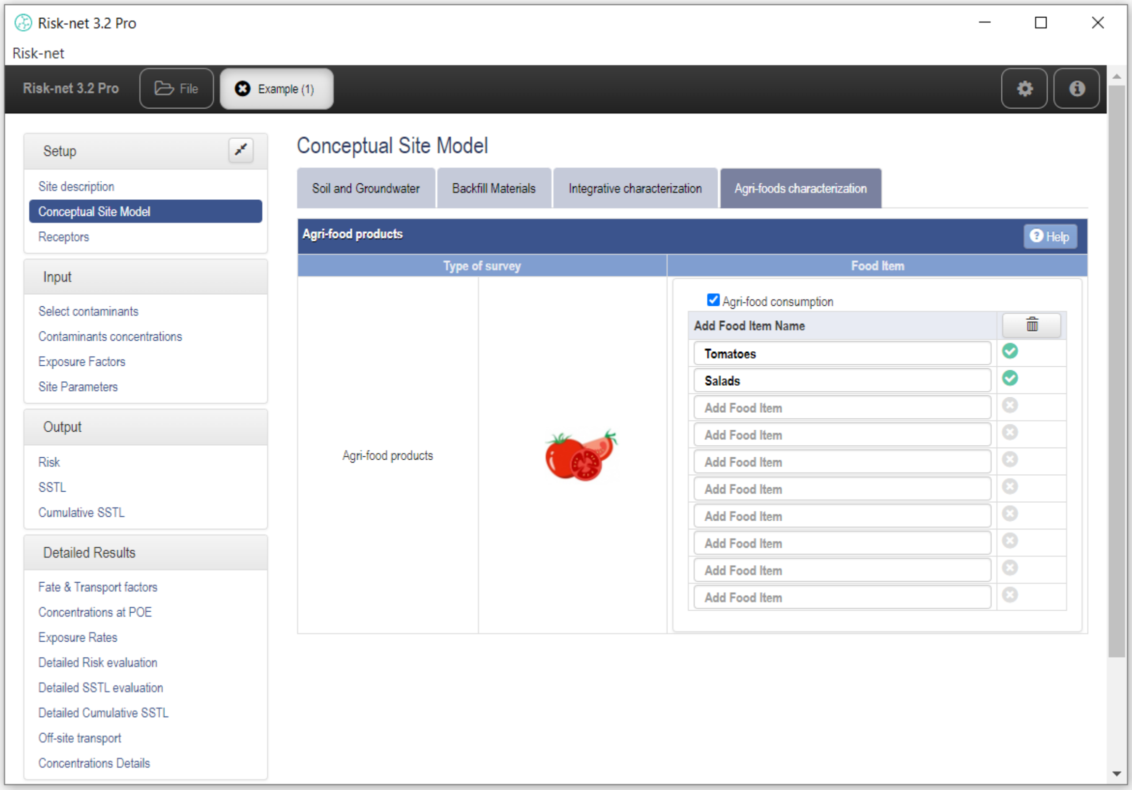
By clicking on the "Integrative characterization" tab the user accesses the screen shown in Figure 9. On this screen, it is possible to select other monitoring data available in terms of ambient air, soil-gas, flux chambers or leaching tests carried out on samples collected ion the surface or subsurface soil. Here the user must also define if the results of this integrative characterization should be used for on-site or off-site exposure.



Type of survey		Type of receptor
Soil-gas survey (outdoor)		☑ On-site receptors ☑ Off-site receptors
Subslab Soil-gas survey		☑ On-site receptors No Off-Site
Flux-Chamber survey (Outdoor)		☑ On-site receptors ☑ Off-site receptors
Flux-Chamber survey (For Indoor)		☑ On-site receptors No Off-Site
Outdoor Air survey		☑ On-site receptors ☑ Off-site receptors
Indoor Air survey		☑ On-site receptors No Off-Site
Leaching test (Surface soil)		☑ POC = 0 m ☑ POC > 0 m

Figure 9. Integrative characterization.

By clicking on the "Agri-foods characterization" tab the user accesses the screen shown in Figure 10. On this screen, the user can activate the risk assessment procedure for food products consumption. Once the checkbox is activated, the user can enter up to 10 food products. To insert the product, the user should enter the name.



☑ Agri-food consumption

Add Food Item Name: Tomatoes ✓

Salads ✓

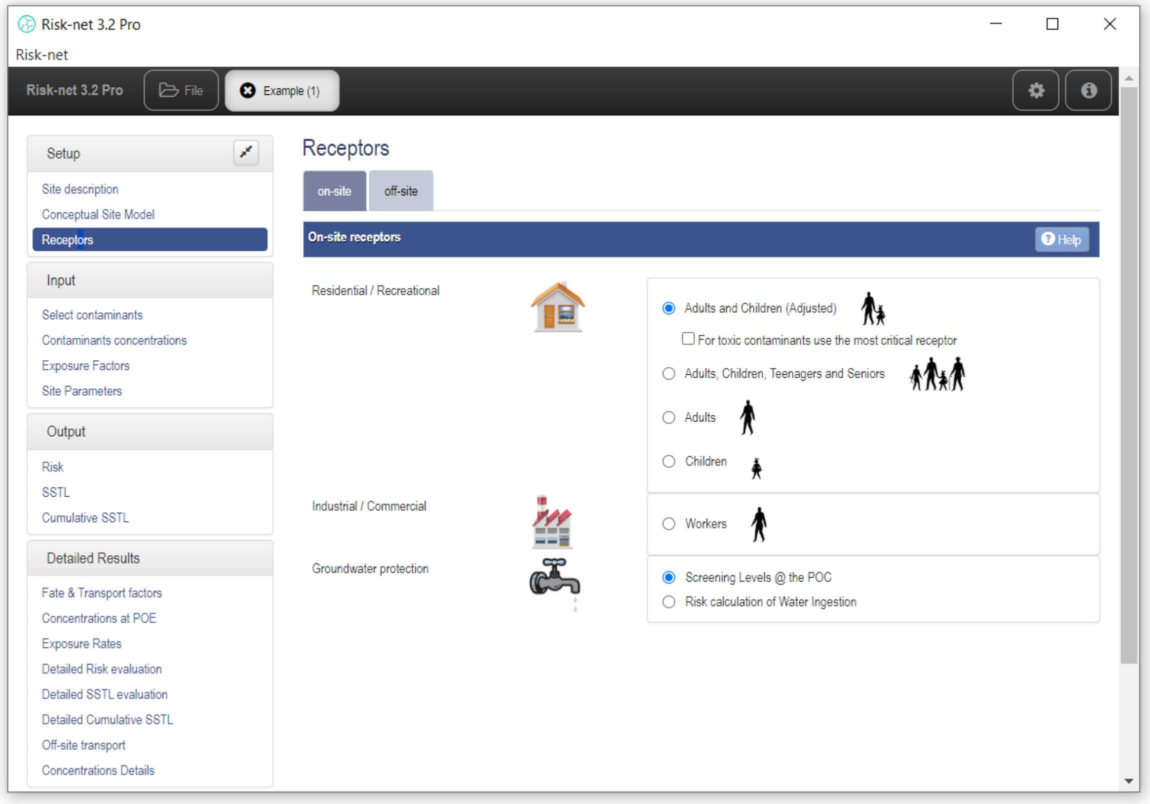
Figure 10. Agri-foods characterization.

RECEPTORS

This screen (Figure 10) is accessed by clicking "Receptors" on the "Setup" menu.
On this screen the user can select the receptors potentially exposed. Namely, the user can select the following receptors:

(a) Adults and Children (Residential or Recreational use);
(b) Adults, Children, Teenagers and Seniors (Residential or Recreational use);
(c) Adult (Residential or Recreational use): Adult with a full grown body weight and skin surface area.
(d) Child (Residential or Recreational use): Children (default age 6 and under), with a low body weight and small skin surface area.
(e) Adult (Commercial or Industrial use): Models an adult working at a full-time job.

In the case of option (a) and (b) for carcinogenic substances, an average calculation of the different receptors is carried out, while for toxic substances the user can decide whether to consider a Child (default option) or to select the most critical receptor according to the selected exposure parameters.



Residential / Recreational

● Adults and Children (Adjusted)

☐ For toxic contaminants use the most critical receptor

○ Adults, Children, Teenagers and Seniors

○ Adults

○ Children

Industrial / Commercial

○ Workers

Groundwater protection

● Screening Levels @ the POC

○ Risk calculation of Water Ingestion

Figure 11. Receptors.

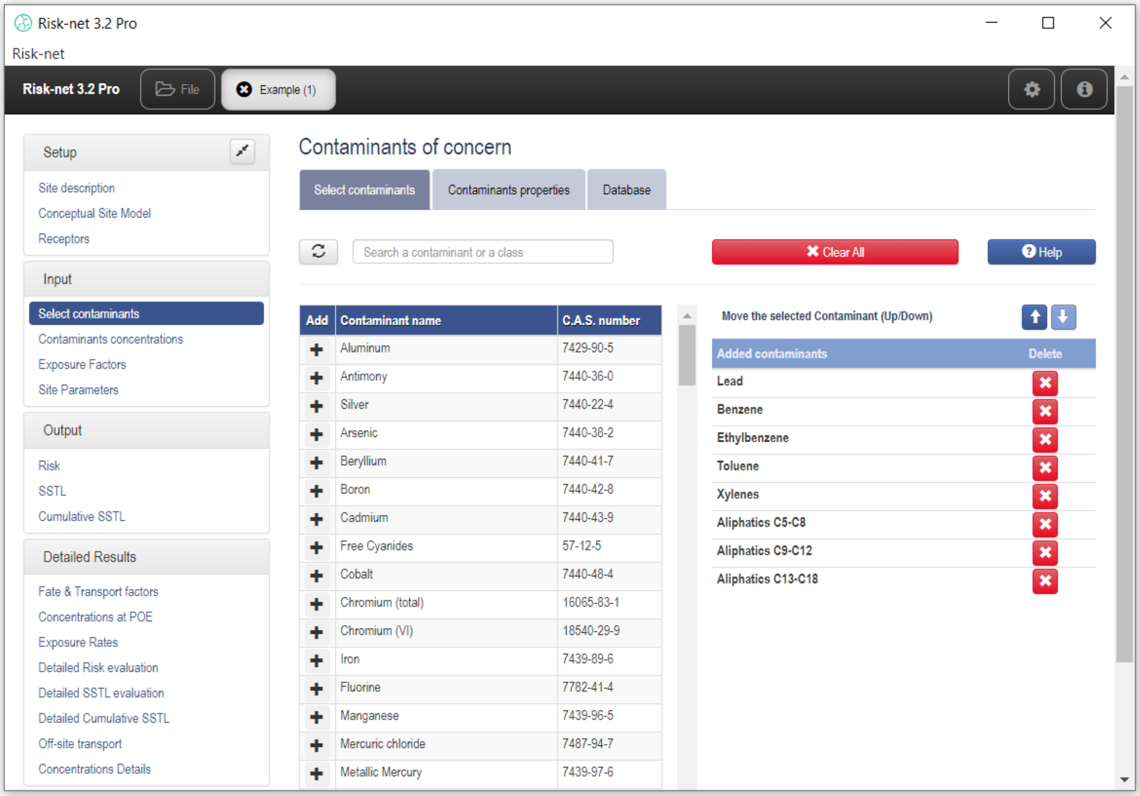
If the leaching or groundwater transport was activated in the conceptual site model, on this screen the user must select whether to calculate the risk for the groundwater resource (i.e. comparison with MCLs) or the health risk associated to the ingestion of water.
The aforementioned operations must be carried out separately for on-site and off-site receptors. Note that in the case in which exposure pathways for on-site or off-site targets are not active, the relative tabs are obscured.

INPUT

CONTAMINANTS OF CONCERN

This screen (Figure 12) is accessed by clicking "Select Contaminants" on the "Input" menu.

Select Contaminants. On this screen, the user can select the chemicals that are of concern for the analysis. The software includes a Chemical Toxicity database pre-loaded with the Italian database issued by ISS-INAIL.



Add	Contaminant name	C.A.S. number
+	Aluminum	7429-90-5
+	Antimony	7440-36-0
+	Silver	7440-22-4
+	Arsenic	7440-38-2
+	Beryllium	7440-41-7
+	Boron	7440-42-8
+	Cadmium	7440-43-9
+	Free Cyanides	57-12-5
+	Cobalt	7440-48-4
+	Chromium (total)	16065-83-1
+	Chromium (VI)	18540-29-9
+	Iron	7439-89-6
+	Fluorine	7782-41-4
+	Manganese	7439-96-5
+	Mercuric chloride	7487-94-7
+	Metallic Mercury	7439-97-6

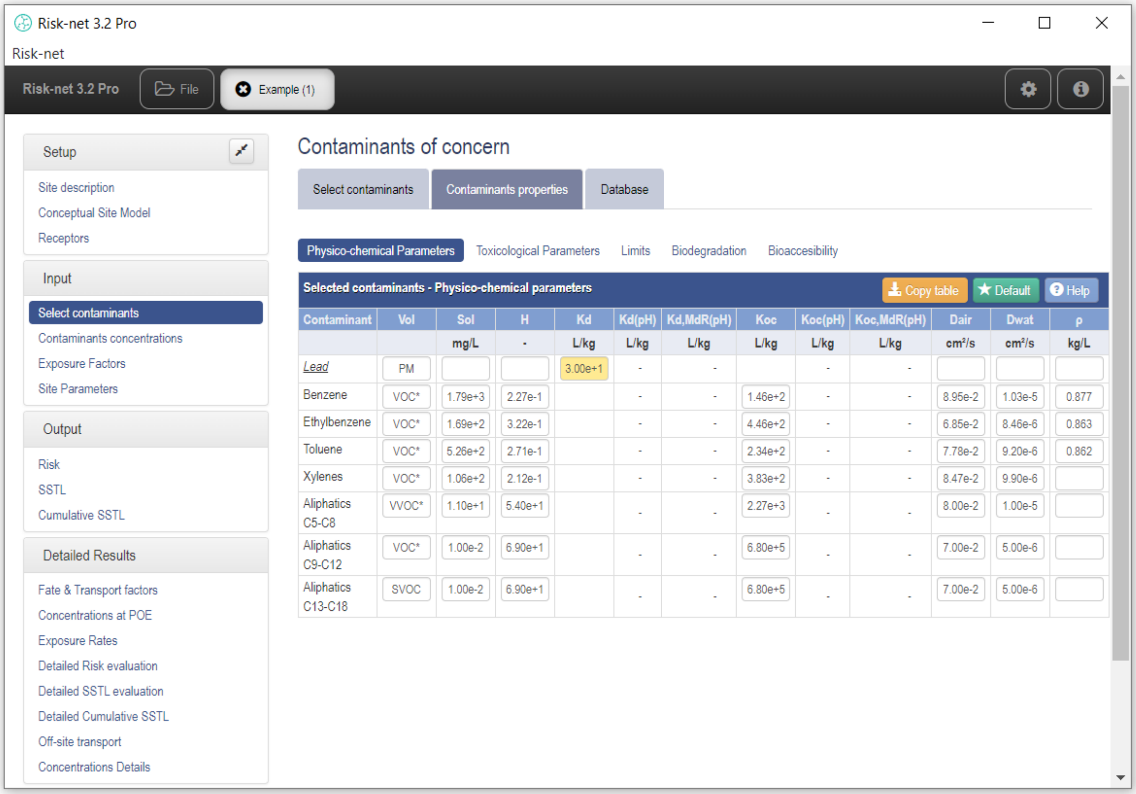
Added contaminants	Delete
Lead	✖
Benzene	✖
Ethylbenzene	✖
Toluene	✖
Xylenes	✖
Aliphatics C5-C8	✖
Aliphatics C9-C12	✖
Aliphatics C13-C18	✖

Figure 12. Select Contaminants.

To add the chemical of concern the user has to click on the + button placed on the left of the contaminant name (the selected contaminants are highlighted with the symbol ☑). To speed up the selection of contaminants it is possible to use the "Search for a contaminant" filter at the top left of the screen (a search can be made not only on the basis of the name of the contaminant but also of the CAS number, contaminant class, volatility). The button

↻ allows the user to cancel the filter used to search for a contaminant. The selected contaminants are added in the window located to the right of the screen. Here the user can change the order of index contaminants (selecting the contaminant of interest and using the up and down arrows ⬆⬇) or remove one of the selected contaminants with the button ✖. The "Clear All" button allows you to quickly remove all previously entered contaminants.

Contaminants properties. On this screen, the user can check and modify the chemico-physical properties of the contaminants of concern.



Selected contaminants - Physico-chemical parameters

Contaminant	Vol	Sol	H	Kd	Kd(pH)	Kd,MdR(pH)	Koc	Koc(pH)	Koc,MdR(pH)	Dair	Dwat	ρ
		mg/L	-	L/kg	L/kg	L/kg	L/kg	L/kg	L/kg	cm²/s	cm²/s	kg/L
Lead	PM			3.00e+1	-	-		-	-			
Benzene	VOC*	1.79e+3	2.27e-1		-	-	1.46e+2	-	-	8.95e-2	1.03e-5	0.877
Ethylbenzene	VOC*	1.69e+2	3.22e-1		-	-	4.46e+2	-	-	6.85e-2	8.46e-6	0.863
Toluene	VOC*	5.26e+2	2.71e-1		-	-	2.34e+2	-	-	7.78e-2	9.20e-6	0.862
Xylenes	VOC*	1.06e+2	2.12e-1		-	-	3.83e+2	-	-	8.47e-2	9.90e-6	
Aliphatics C5-C8	VVOC*	1.10e+1	5.40e+1		-	-	2.27e+3	-	-	8.00e-2	1.00e-5	
Aliphatics C9-C12	VOC*	1.00e-2	6.90e+1		-	-	6.80e+5	-	-	7.00e-2	5.00e-6	
Aliphatics C13-C18	SVOC	1.00e-2	6.90e+1		-	-	6.80e+5	-	-	7.00e-2	5.00e-6	

Figure 13. Contaminants properties.

The parameters that are modified compared to the default database are highlighted in yellow and the name of the contaminant is modified in italic and underlined. Note that the values modified in this screen will be considered only for the current simulation. By starting a new simulation, the values defined in the original database will be used.

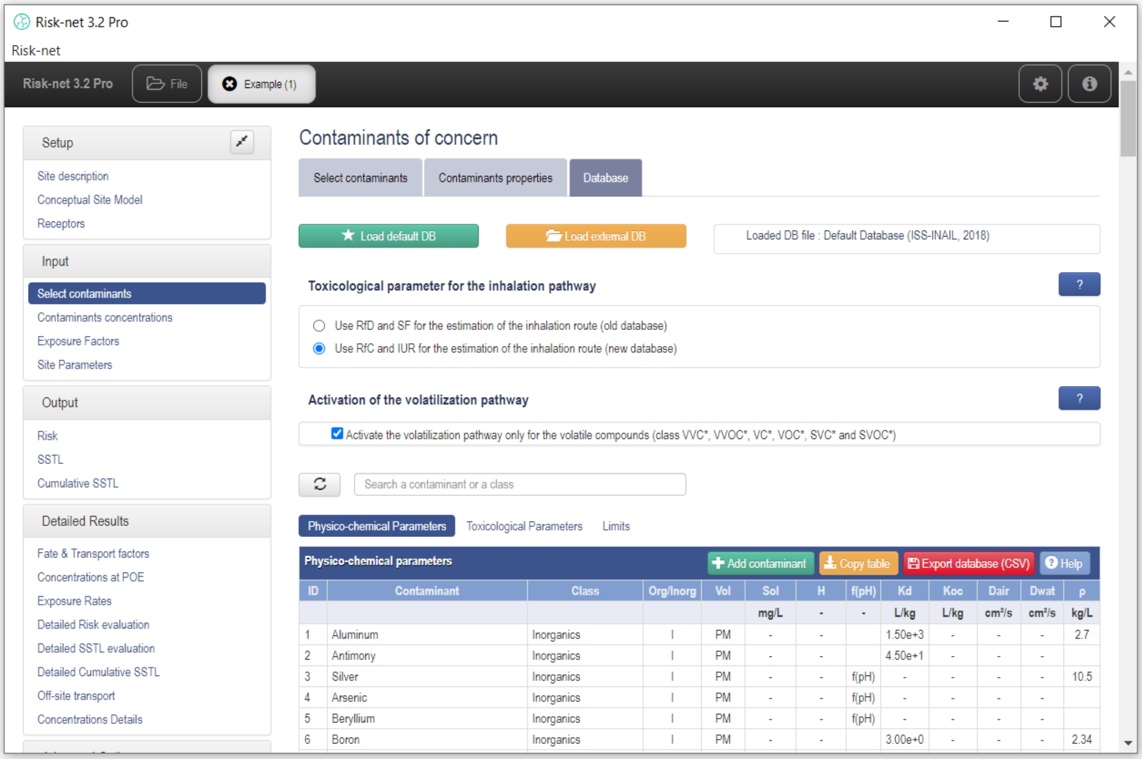
If in the calculation options biodegradation is activated, on this screen the user must also define for the different migration pathways (volatilization, leaching and groundwater transport), the first-order biodegradation constants. Similarly, if in the calculation options it is decided to consider bioaccessibility for calculating the soil ingestion risks on this screen it is necessary to define the bioaccessible fraction of each contaminant. The bioaccessible fraction can vary from a null value (not bioaccessible contaminant) to a value 1 (corresponding to a 100% bioaccessible contaminant).

Database. Here the user can check the contaminants present in the database. By Default, the software implements the Italian ISS-INAIL database (2018). On this screen the user can possibly add new contaminants using the command button ‘Add contaminant’ (in this case the name of the database will be indicated as 'modified' and the name of the modified contaminants will be indicated as '(User)'). On this screen the user can also load external database (button ‘‘Load external DB’) previously created using the CSV file present in the installation folder. Note that the external database loaded in the software is not automatically updated in the case of changes to the external CSV file and therefore in the case where for a simulation it is decided to modify some parameters of the external database it is necessary to repeat the database upload procedure (using the 'Load external DB' button). By clicking on the command button ‘Load default DB’ the software reset the original database present in the software. Note that loading an external database the function of automatic calculation of the partition coefficients Koc and Kd as a function pH value defined on the site is disabled.

On this screen, it is also possible to select the toxicological parameters to be used for the vapor inhalation pathway. Specifically, the user can select to calculate the risks and objectives of reclamation for the route of inhalation using either the reference doses (RfD for non-carcinogens and SF for carcinogens) or the reference concentrations (RfC for non-carcinogens and IUR for carcinogens). The main difference between the two approaches is that the method based on the use of the reference dose (RfD) is based on a re-modulation of the risks as a function of the body weight and the inhalation rate while the method based on the use of reference concentrations (RfC) does not provide for modulations based on body weight and inhalation rate. It is worth noting that the default database present in the software is based on the use of reference concentrations (RfC for non-carcinogens and IUR for carcinogens) and therefore to use the reference dose method with the default database the user must enter the RfD and SF values to be used for the risks and SSTLs calculations.

By default, according to the Italian ISS-INAIL database (2018), the software calculates the indoor and outdoor risks only for some selected contaminants considered sufficiently volatile. These contaminants are indicated in the database with an asterisk (VVOC *, VOC*, SVOC*, VC* and SCV*). Therefore, by default in the software the volatilization pathways in the simulations (Risk calculation and SSTLs) is considered only for these contaminants. This option can be deactivated using the checkbox present on this screen. It should be emphasized that if an external database is loaded, to use this option correctly it is necessary to indicate in the "Vol" column the contaminants considered sufficiently volatile (using the asterisks in the acronyms VVOC*, VOC *, SVOC *, VC * and SCV *).

It is worth noting that to modify the chemico-physical properties of the contaminants of concern the user must enter in the screen ‘Contaminants properties’.



Loaded DB file : Default Database (ISS-INAIL, 2018)

Toxicological parameter for the inhalation pathway

○ Use RfD and SF for the estimation of the inhalation route (old database)
● Use RfC and IUR for the estimation of the inhalation route (new database)

Activation of the volatilization pathway

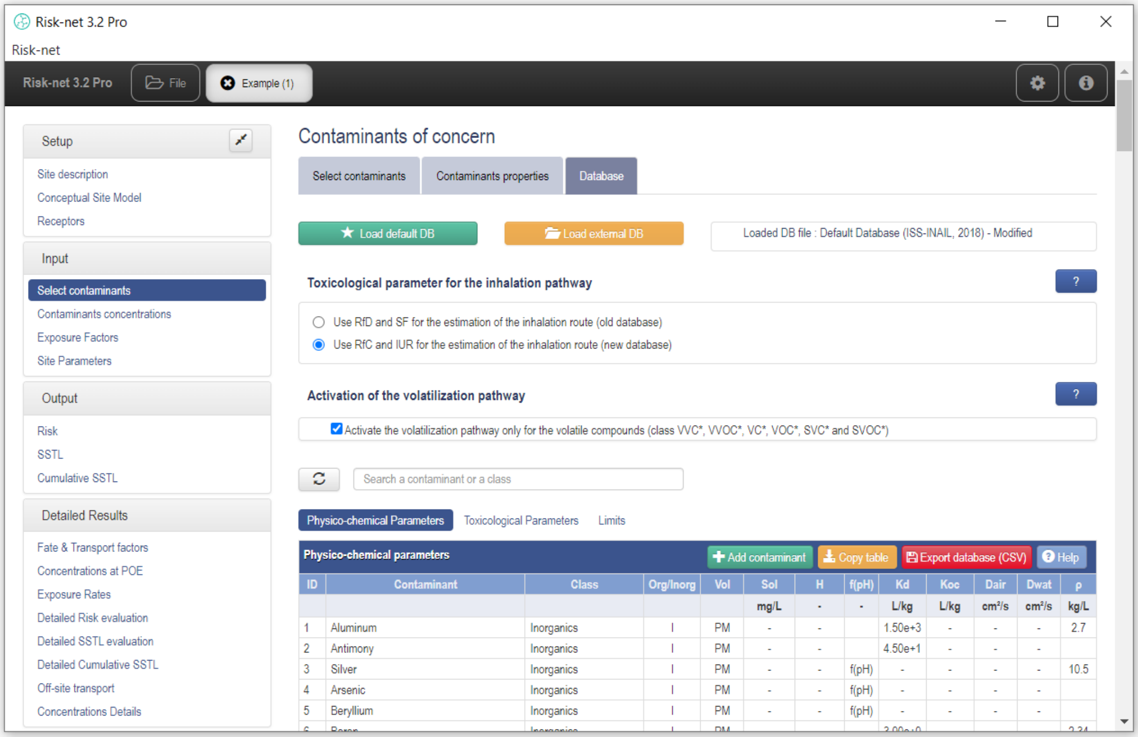
☑ Activate the volatilization pathway only for the volatile compounds (class VVC*, VVOC*, VC*, VOC*, SVC* and SVOC*)

Physico-chemical parameters

ID	Contaminant	Class	Org/Inorg	Vol	Sol	H	f(pH)	Kd	Koc	Dair	Dwat	ρ
					mg/L	-	-	L/kg	L/kg	cm²/s	cm²/s	kg/L
1	Aluminum	Inorganics	I	PM	-	-		1.50e+3	-	-	-	2.7
2	Antimony	Inorganics	I	PM	-	-		4.50e+1	-	-	-	
3	Silver	Inorganics	I	PM	-	-	f(pH)	-	-	-	-	10.5
4	Arsenic	Inorganics	I	PM	-	-	f(pH)	-	-	-	-	
5	Beryllium	Inorganics	I	PM	-	-	f(pH)	-	-	-	-	
6	Boron	Inorganics	I	PM	-	-		3.00e+0	-	-	-	2.34

Figure 14. Database.

Note that by changing the database for a simulation in progress, the previously selected contaminants are replaced with those having the same ID number in the new database. If in the new database a previously selected contaminant is not present (i.e. in the new database there is no contaminant with the same ID), the software for that specific contaminant, maintains the chemical-physical and toxicological parameters present in the database used in the old simulation.



Contaminants of concern

Loaded DB file : Default Database (ISS-INAIL, 2018) - Modified

Toxicological parameter for the inhalation pathway

○ Use RfD and SF for the estimation of the inhalation route (old database)
● Use RfC and IUR for the estimation of the inhalation route (new database)

Activation of the volatilization pathway

☑ Activate the volatilization pathway only for the volatile compounds (class VVC*, VVOC*, VC*, VOC*, SVC* and SVOC*)

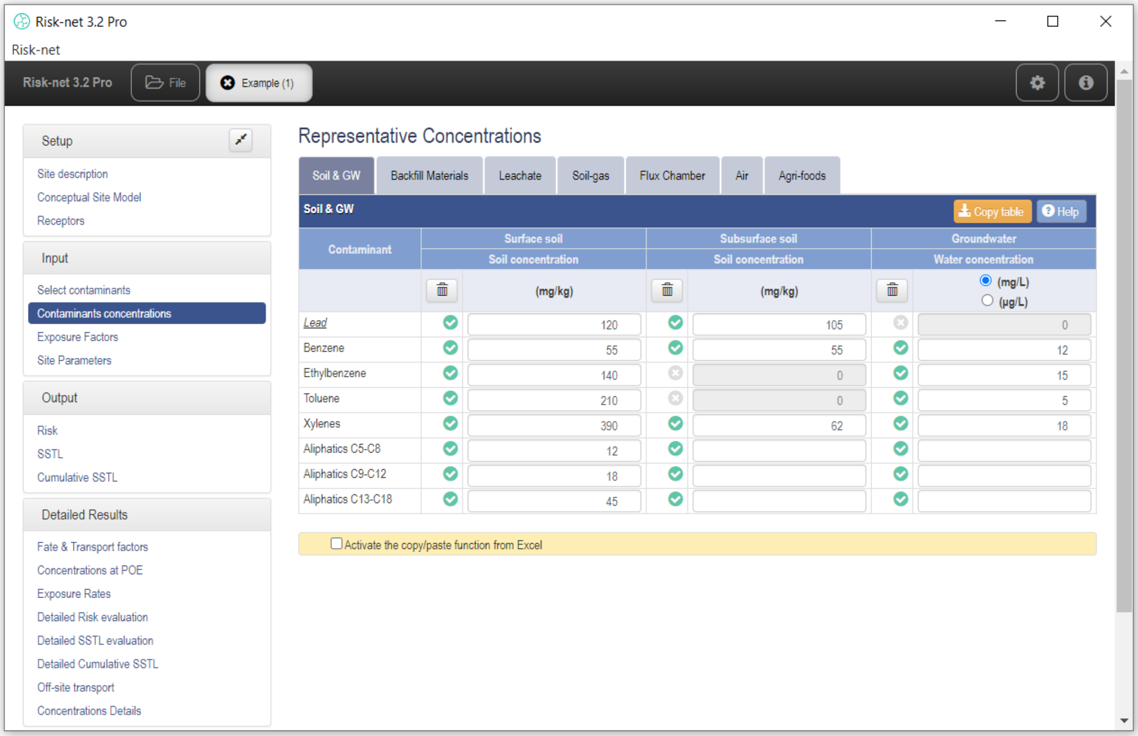
Physico-chemical parameters

ID	Contaminant	Class	Org/Inorg	Vol	Sol	H	f(pH)	Kd	Koc	Dair	Dwat	ρ
					mg/L	-	-	L/kg	L/kg	cm²/s	cm²/s	kg/L
1	Aluminum	Inorganics	I	PM	-	-		1.50e+3	-	-	-	2.7
2	Antimony	Inorganics	I	PM	-	-		4.50e+1	-	-	-	
3	Silver	Inorganics	I	PM	-	-	f(pH)	-	-	-	-	10.5
4	Arsenic	Inorganics	I	PM	-	-	f(pH)	-	-	-	-	
5	Beryllium	Inorganics	I	PM	-	-	f(pH)	-	-	-	-	

Figure 15. Example of new contaminants in the Database.

SOURCE ZONE CONCENTRATION

This screen (Figure 16) is accessed by clicking "Contaminants concentrations" on the "Input" menu. Here, the user can enter the concentrations measured for each matrix that has been activated in the conceptual site model (CSM). If advanced characterization data are available (e.g. eluate, soil-gas, flux-chamber or air) and they have been activated in the ‘Integrative characterization’ of the ‘Conceptual Site Model’ screen, the user can also enter these concentrations. In the event that a contaminant has been detected only in one medium, to deselect it from the other source media where the contaminant is not of concern, it is sufficient to set a null concentration (zero) and the contaminant will be automatically deselected (the green check to the left of the contaminant’s name becomes a gray 'x' as shown in the figure for Ethylbenzene in the subsurface soil). If the user does not enter any value, the contaminant will be considered active but it will not possible to calculate the risks. To paste data from excel the user can activate the 'Enable Copy / Paste From Excel' box present on this screen. In this case, the user can copy the entire column from excel and copy into the table by selecting the first row of the matrix on which to paste the data. This operation must be repeated for each source activated by the user. The contaminants for which the chemico-physical and/or toxicological properties have been modified, are underlined and in italic.



Representative Concentrations

Soil & GW

Contaminant	Surface soil		Subsurface soil		Groundwater	
	Soil concentration		Soil concentration		Water concentration	
		(mg/kg)		(mg/kg)		● (mg/L) ○ (µg/L)
Lead	✓	120	✓	105	⊗	0
Benzene	✓	55	✓	55	✓	12
Ethylbenzene	✓	140	⊗	0	✓	15
Toluene	✓	210	⊗	0	✓	5
Xylenes	✓	390	✓	62	✓	18
Aliphatics C5-C8	✓	12	✓		✓	
Aliphatics C9-C12	✓	18	✓		✓	
Aliphatics C13-C18	✓	45	✓		✓	

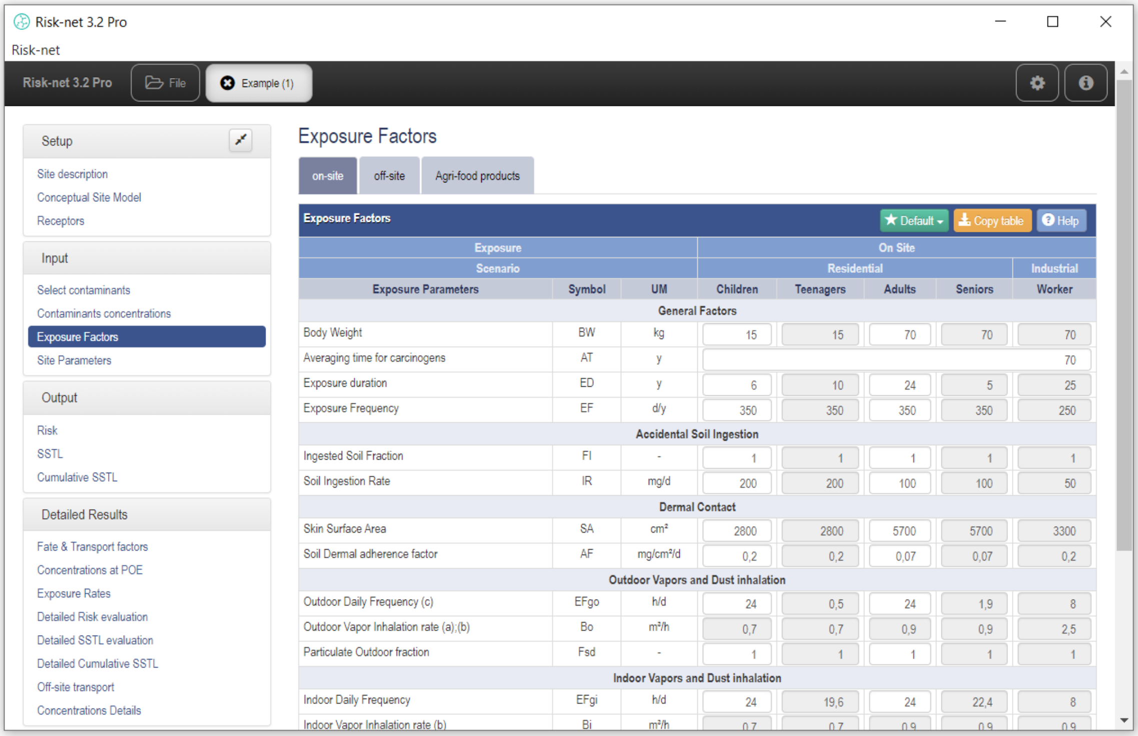
☐ Activate the copy/paste function from Excel

Figure 16. Source Concentration.

For the concentrations in groundwater and in the eluate the user can choose whether to enter the data expressed as µg/L or mg/L (the software will automatically convert the concentrations to the unit of measurement required in the calculations). In a similar way the user can enter the concentration data related to soil-gas, flow chambers and in the air as µg /m^3 or mg/m^3.

EXPOSURE FACTORS

This screen (Figure 16) is accessed by clicking "Exposure Factors" on the "Input" menu. On this screen, the user must enter appropriate exposure factors for each complete pathway. By default, this section contains the values corresponding to Italian guidelines (ISPRA, 2008). There are different exposure factor columns representing the different types of receptors that can be modeled with the software. These receptor types allow the user to calculate baseline risks and cleanup levels based on different physical (e.g., skin area, body weight, etc.) and exposure-related (e.g., soil ingestion rate, inhalation rate, etc.) parameters.



Exposure			On Site				
Scenario			Residential				Industrial
Exposure Parameters	Symbol	UM	Children	Teenagers	Adults	Seniors	Worker
General Factors							
Body Weight	BW	kg	15	15	70	70	70
Averaging time for carcinogens	AT	y	70				
Exposure duration	ED	y	6	10	24	5	25
Exposure Frequency	EF	d/y	350	350	350	350	250
Accidental Soil Ingestion							
Ingested Soil Fraction	FI	-	1	1	1	1	1
Soil Ingestion Rate	IR	mg/d	200	200	100	100	50
Dermal Contact							
Skin Surface Area	SA	cm²	2800	2800	5700	5700	3300
Soil Dermal adherence factor	AF	mg/cm²/d	0,2	0,2	0,07	0,07	0,2
Outdoor Vapors and Dust inhalation							
Outdoor Daily Frequency (c)	EFgo	h/d	24	0,5	24	1,9	8
Outdoor Vapor Inhalation rate (a);(b)	Bo	m³/h	0,7	0,7	0,9	0,9	2,5
Particulate Outdoor fraction	Fsd	-	1	1	1	1	1
Indoor Vapors and Dust inhalation							
Indoor Daily Frequency	EFgi	h/d	24	19,6	24	22,4	8
Indoor Vapor Inhalation rate (b)	Bi	m³/h	0,7	0,7	0,9	0,9	0,9

Figure 17. Exposure Factors.

To speed up the compilation process, the software requires only the parameters actually used in the calculations for the specific case based on the active exposure pathway and selected targets. In particular, the grey cells are the data not required, while the data to be entered are the white cells. The modified values are highlighted in yellow. With the 'Default' button it is possible to reset the default values suggested by the Italian guidelines (Table 2).

Table 2. Default values implemented in the software (ISPRA, 2008).

Scenario			Residential				Industrial
Exposure Parameters	Symbol	UM	Children	Teenagers	Adults	Seniors	Worker
General Factors							
Body Weight	BW	kg	15	15	70	70	70
Averaging time for carcinogens	AT	y	70				
Exposure duration	ED	y	6	10	24	5	25
Exposure Frequency	EF	d/y	350	350	350	350	250
Accidental Soil Ingestion							
Ingested Soil Fraction	FI	-	1	1	1	1	1
Soil Ingestion Rate	IR	mg/d	200	200	100	100	50
Dermal Contact							
Skin Surface Area	SA	cm²	2800	2800	5700	5700	3300
Soil Dermal adherence factor	AF	mg/cm²/d	0.2	0.2	0.07	0.07	0.2

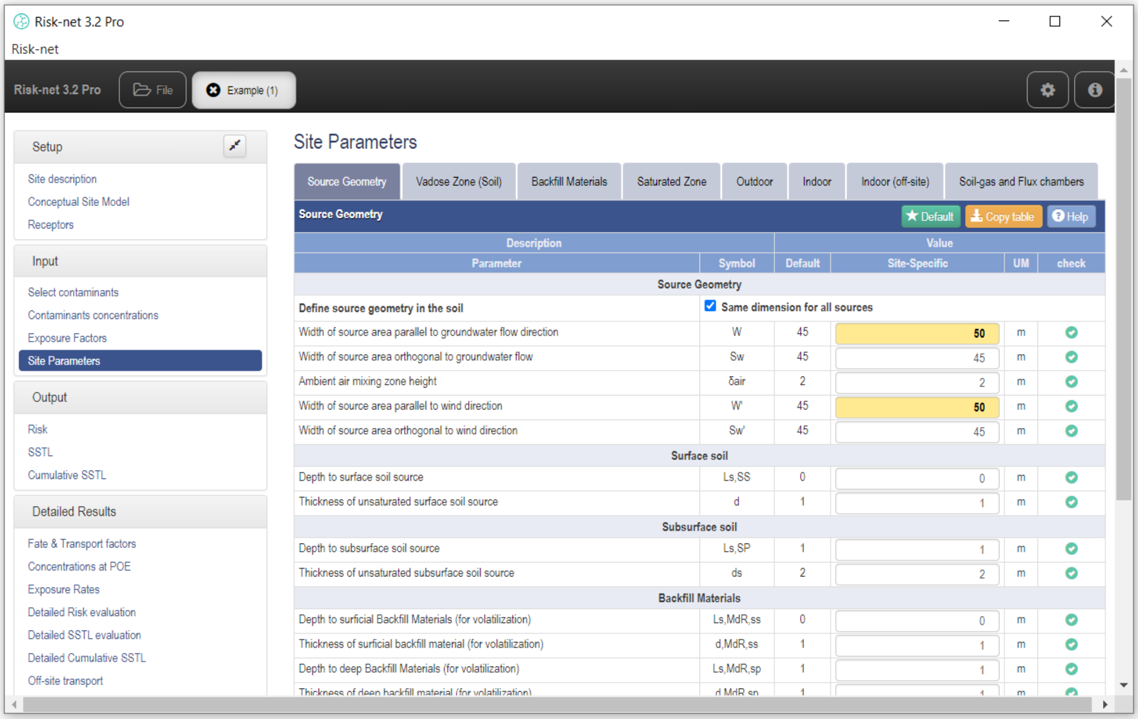
Scenario			Residential				Industrial
Exposure Parameters	**Symbol**	**UM**	**Children**	**Teenagers**	**Adults**	**Seniors**	**Worker**
Outdoor Vapors and Dust inhalation							
Outdoor Daily Frequency	EFgo	h/d	24	0.5	24	1.9	8
Outdoor Vapor Inhalation rate	Bo	m³/h	0.7	0.7	0.9	0.9	2.5
Particulate Outdoor fraction	Fsd	-	1	1	1	1	1
Indoor Vapors and Dust inhalation							
Indoor Daily Frequency	EFgi	h/d	24	19.6	24	22.4	8
Indoor Vapor Inhalation rate	Bi	m³/h	0.7	0.7	0.9	0.9	0.9
Particulate indoor fraction	Fi	-	1	1	1	1	1
Water Ingestion							
Water Rate Ingestion	IRw	L/d	1	1	2	2	1

SITE PARAMETERS

This screen (Figure 16) is accessed by clicking "Site Parameters" on the "Input" menu. In this section, the user provides the site-specific parameters required for the application of the fate and transport models selected. Specifically, the user must enter the following parameters:

(a) **Source Geometry**: source geometry in soil and groundwater.
(b) **Vadose zone**: soil properties, rainfall, infiltration rate, fraction of organic carbon, pH, etc.
(c) **Backfill Materials**: BM properties, infiltration rate, fraction of organic carbon, pH, etc.
(d) **Saturated zone**: physical characteristics, fraction of organic carbon and other transport properties.
(e) **Outdoor**: wind speed, dispersion in air, particulate emissions, etc.
(f) **Indoor**: building geometry and properties, air exchange rate, indoor/outdoor differential pressure, etc.
(g) **Soil-gas and Flux Chambers**: probe depth, chamber surface, etc.

By default, the software contains the default values suggested by the Italian ISPRA guidelines (2008). To speed up the compilation process, the software requires only the parameters actually used in the calculations for the specific case based on the active exposure pathway and selected targets. In particular, the grey cells are the data not required, while the data to be entered are the white cells. The modified values are highlighted in yellow.



Description		Value			
Parameter	Symbol	Default	Site-Specific	UM	check
Source Geometry					
Define source geometry in the soil	☑ **Same dimension for all sources**				
Width of source area parallel to groundwater flow direction	W	45	**50**	m	✓
Width of source area orthogonal to groundwater flow	Sw	45	45	m	✓
Ambient air mixing zone height	δair	2	2	m	✓
Width of source area parallel to wind direction	W'	45	**50**	m	✓
Width of source area orthogonal to wind direction	Sw'	45	45	m	✓
Surface soil					
Depth to surface soil source	Ls,SS	0	0	m	✓
Thickness of unsaturated surface soil source	d	1	1	m	✓
Subsurface soil					
Depth to subsurface soil source	Ls,SP	1	1	m	✓
Thickness of unsaturated subsurface soil source	ds	2	2	m	✓
Backfill Materials					
Depth to surficial Backfill Materials (for volatilization)	Ls,MdR,ss	0	0	m	✓
Thickness of surficial backfill material (for volatilization)	d,MdR,ss	1	1	m	✓
Depth to deep Backfill Materials (for volatilization)	Ls,MdR,sp	1	1	m	✓
Thickness of deep backfill material (for volatilization)	d,MdR,sp	1	1	m	✓

Figure 18. Site Parameters.

The options that can be activated in these screens are briefly described below.

Same dimension for all sources. By default, in the software the same geometry of the source is assumed for the different source media selected in the conceptual site model (e.g. surface soil, subsurfcae soil and groundwater). If the dimension of the sources is different, it is possible to uncheck the checkbox "Same dimension for all sources". In this case it is possible to enter the specific geometric parameters for each environmental compartment.

Lens present. By activating this option, the user can take into account in the calculation of risks and SSTLs for outdoor and indoor volatilization from subsurface soil and groundwater for the presence of a geological vapor barrier (e.g. clay lens) placed between the source of contamination and the ground surface. In particular, by activating the user must define the thickness, porosity and water content of the lens. These parameters are required to estimate molecular diffusion through this layer (for more details see the equations in the appendix).

Soil texture. For the soil parameter the user can choose the predominant soil texture from the drop-down menu and use the literature values indicated by Italian ISPRA guidelines ISPRA (2008) or enter site-specific data (or other literature values) by selecting the "Site-specific" item from the drop-down menu. Table 3 shows the default data implemented in the software as a function of the soil texture.

Table 3. Default soil parameters values implemented in the software (ISPRA, 2008).

USDA Soil Texture	**K_{sat}**	**θ_r**	**θ_e**	**θ_a**	**θ_w**	**θ_{acap}**	**θ_{wcap}**	**h_{cap}**
	m/s	**-**	**-**	**-**	**-**	**-**	**-**	**cm**
SAND	8.25E-05	0.045	0.385	0.317	0.068	0.055	0.33	10
LOAMY SAND	4.05E-05	0.057	0.353	0.25	0.103	0.035	0.318	18.8
SANDY LOAM	1.23E-05	0.065	0.345	0.151	0.194	0.057	0.288	25
SANDY CLAY LOAM	3.64E-06	0.1	0.29	0.112	0.178	0.042	0.248	25.9
LOAM	2.89E-06	0.078	0.352	0.139	0.213	0.035	0.317	37.5
SILT LOAM	1.25E-06	0.067	0.383	0.128	0.255	0.086	0.297	68.2
CLAY LOAM	7.22E-07	0.095	0.315	0.115	0.2	0.027	0.288	46.9
SILTY CLAY LOAM	1.94E-07	0.089	0.341	0.095	0.246	0.024	0.317	133.9
SILTY CLAY	5.56E-08	0.07	0.29	0.016	0.274	0.008	0.282	192
SILT	6.94E-07	0.034	0.426	0.148	0.278	0.043	0.383	163
SANDY CLAY	3.33E-07	0.1	0.28	0.052	0.228	0.028	0.252	30
CLAY	5.56E-07	0.068	0.312	0.008	0.304	0.004	0.308	81.5

USDA. To select the representative soil texture, the user can use the function implemented in the software which, based on the percentage of sand, silt and clay, calculates the representative texture according to the USDA classification. In particular, by clicking on the "USDA" button the mass percentage of sand and silt is requested (the percentage of clay is calculated as a complement to 100) and by clicking the "Calculate USDA class" button the reference texture is identified. To select the calculated class, press the “Select calculated class” button.

Soil Infiltration Rate. The user can choose whether to calculate this parameter according to the rainfall and the type of soil selected (using the empirical equations proposed by the ISPRA document (2008) and reported in the appendix of the manual) or enter it manually.

HDPE or low-permeability layer present. By activating this option, the user can define the characteristics of an HDPE sheet present above the source of contamination or of a low-permeability layer between the source and the aquifer. These data are used in the software to calculate the effective soil infiltration rate for the leaching pathway. The equations used for these estimates are reported in the appendix and refer to the models described in the guidelines on risk analysis for landfills prepared by ISPRA (2005). Note that the HDPE sheet and the low permeability layer inserted in this screen are used exclusively for the leaching pathway (i.e. data not considered for the volatilization pathway).

Select the type of backfill materials. For the specific characteristics of the type of backfill materials found on the site, the user can choose, from the drop-down menu, whether to use the data indicated in the SNPA Guidelines 46bis/2023 or define site-specific data by selecting the item from the drop-down menu “Site-Specific”. Table 4 shows the data implemented in the software relating to the different types of backfill material in accordance with the provisions of the SNPA 46bis/2023 Guidelines.

Table 4. Backfill material parameters values implemented in the software.

Backfill Material	**K_{sat}**	**θ_r**	**θ_e**	**θ_a**	**θ_w**	**ρ_{MdR}**	**pH_{MdR}**
	m/s	**-**	**-**	**-**	**-**	**kg/L**	**-**
Fly Ash	5.0E-07	0.047	0.494	0.307	0.187	0.7	8
Bottom Ash	4.10E-05	0.025	0.553	0.477	0.076	1.2	8
Incineration waste	1.00E-04	0.049	0.401	0.285	0.116	1.0	8
Ashes	4.10E-04	0.02	0.355	0.300	0.055	1.5	8
C&D	1.00E-04	0.013	0.384	0.352	0.032	2.4	6.8
Materials with acidic inorganic substances	2.0E-06	0.045	0.385	0.317	0.068	1.7	4.9
Materials with plastics and/or wood	2.0E-06	0.045	0.385	0.317	0.068	1.0	6.8
Other types	2.0E-06	0.045	0.385	0.317	0.068	1.7	6.8

Calculation of diffusion coefficients due to volatilization from groundwater. If pathways pertaining to backfill materials are chosen in the conceptual model, within the "Backfill Materials" screen, you can enable the checkbox labeled "Use Backfill Material Parameters." This allows for the utilization of parameters from the capillary fringe and unsaturated zone defined for the backfill materials in the calculation of diffusion coefficients for the volatilization pathway (both outdoor and indoor) from groundwater, if activated within the conceptual model. This option is applicable when the backfill material horizon significantly influences a substantial portion of the unsaturated zone, extending towards the vicinity of the saturated zone.

Effective infiltration calculation in Backfill Materials. By activating the checkbox "Consider Ieff used for soils," it is possible to use the estimated effective infiltration value for soils. This option should be activated, as indicated by SNPA Guidelines 46bis/2023, if there are less permeable horizons within, above, and/or below the Backfill materials with a certain thickness and spatial continuity within the unsaturated zone.

Selection of Saturated Zone Texture. Considering the specific characteristics of the soil type in the saturated zone at the site, users can choose from the drop-down menu whether to utilize the data provided in the ISPRA document (2008) as outlined in SNPA Guidelines 46bis/2023 (in the presence of Backfill Material in the saturated zone), or define site-specific data by selecting "Site-Specific" from the drop-down menu. Table 5 displays the data implemented in the software pertaining to various soil types and Backfill Materials.

Table 5. Specific parameter values for some types of soil and anthropogenic material.

Texture	K_{sat}	θ_e
	m/s	**-**
SAND	8.25E-05	0.385
LOAMY SAND	4.05E-05	0.353
SANDY LOAM	1.23E-05	0.345
SANDY CLAY LOAM	3.64E-06	0.29
LOAM	2.89E-06	0.352
SILT LOAM	1.25E-06	0.383
CLAY LOAM	7.22E-07	0.315
SILTY CLAY LOAM	1.94E-07	0.341
SILTY CLAY	5.56E-08	0.29
SILT	6.94E-07	0.426
SANDY CLAY	3.33E-07	0.28
CLAY	5.56E-07	0.312
Fly Ash	5.0E-07	0.494
Bottom Ash	4.10E-05	0.553
Incineration waste	1.00E-04	0.401
Ashes	4.10E-04	0.355
C&D	1.00E-04	0.384

Dispersivity in groundwater. The user can choose whether to enter them manually or calculate them based on the distance from the point of compliance (for more details, see the equations in the appendix).

Calculate wind speed. The wind speed to be entered into the software must refer to the height of the mixing zone in the air (which by default is set equal to 2 m height from the ground surface). If the data available for wind speed refer to a different height (e.g. 10 m) it is possible to calculate the expected value at the height of interest using the empirical equations reported in the ISPRA document (see appendix of the manual).

Air dispersion coefficient. The user can choose whether to enter them manually or calculate them according to the stability class and the distance of the off-site receptors using the empirical equations reported by Briggs (1973).

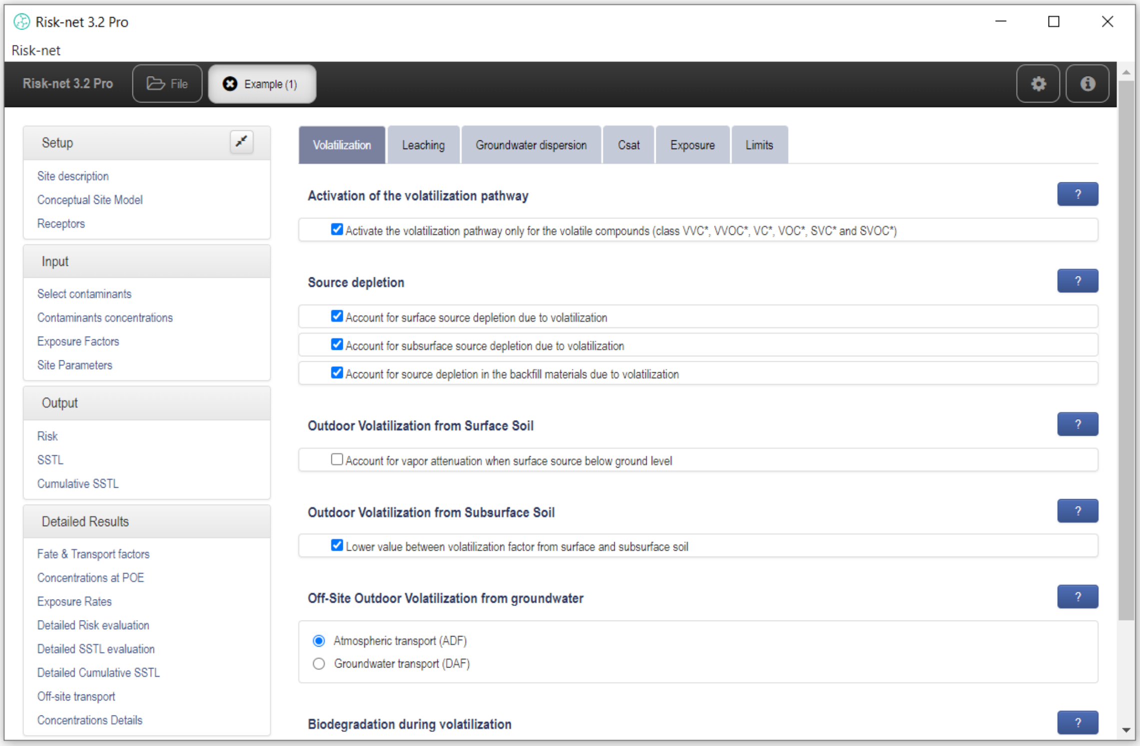
Pressure difference between outdoor and indoor. If the convective transport of vapors within the indoor environment is relevant at the site of concern, the user must enter a value of "Δp" greater than zero and enter the additional parameters required.

Site-specific indoor convective flow. If available, the user can enter a site-specific value of the convective airflow entering the building.

Empirical soil-gas attenuation factor of soil-gas. For soil-gas data, instead of the analytical models implemented in the software, by activating this option the user can enter empirical attenuation factors to be used for the calculation of the risks for the indoor and outdoor vapor inhalation pathway.

MODEL OPTIONS

By default, Risk-net implements the equations and calculation criteria outlined in the Italian ISPRA guidelines (2008). However, to make the tool more versatile it is possible to activate and define some supplementary calculation options. To view or modify the active options, the user must access the "Model options" from the "Advanced Options" menu (Figure 19). These options are divided into the following tabs: "Volatilization", "Leaching", "Groundwater dispersion", "Csat", "Exposure" and "Limits".



Activation of the volatilization pathway

☑ Activate the volatilization pathway only for the volatile compounds (class VVC*, VVOC*, VC*, VOC*, SVC* and SVOC*)

Source depletion

☑ Account for surface source depletion due to volatilization

☑ Account for subsurface source depletion due to volatilization

☑ Account for source depletion in the backfill materials due to volatilization

Outdoor Volatilization from Surface Soil

☐ Account for vapor attenuation when surface source below ground level

Outdoor Volatilization from Subsurface Soil

☑ Lower value between volatilization factor from surface and subsurface soil

Off-Site Outdoor Volatilization from groundwater

● Atmospheric transport (ADF)

○ Groundwater transport (DAF)

Biodegradation during volatilization

Figure 19. Site Parameters.

The different options are briefly described below.

VOLATILIZATION

Source depletion. By activating this option, the software accounts, through a mass balance, for the source depletion. In particular, the outdoor and indoor volatilization is calculated by selecting, for each contaminant, the smaller value obtained from the fate and transport factor and the mass balance equation. For more details, readers are directed to the appendix with the description of the equations implemented in the software.

Outdoor Volatilization from Surface Soil. By activating this option, if the source in the surface soil is at some depth below the ground surface, the volatilization factor is calculated by employing the model for the subsurface soil.

Outdoor Volatilization from Subsurface Soil. By activating this option, for contaminated subsurface soil, the software checks if the volatilization estimated by the model is higher than the one expected from the surface soil (and in this case select the latter as representative of the volatilization from soil).

Off-Site Outdoor Volatilization from groundwater. For contaminated groundwater, the off-site transport of vapors can be modelled considering volatilization from the source and dispersion in atmosphere (ADF) or groundwater transport (DAF) and volatilization.

Biodegradation during volatilization. By activating this option, it is possible to account for aerobic biodegradation of vapors in the subsurface. In this case, the user must define the biodegradation kinetic constant in the screen with the chemical properties of selected contaminants and the thickness of the aerobic zone in the screen with the definition of site-specific parameters.

LEACHING

Source depletion. By activating this option, the software accounts, through a mass balance, for the source depletion. In particular, the leaching factor is calculated by selecting, for each contaminant, the smaller value obtained from the fate and transport factor and the mass balance equation.

Soil Attenuation Model (SAM). The SAM (Connor, 1997) corrects the equilibrium soil leachate concentration for the effect of sorptive mass loss as the leachate percolates downward toward the underlying water-bearing unit. For the SAM, the affected soil zone is characterized as a finite source mass equivalent to the affected soil mass times the representative constituent concentration. Prior to reaching groundwater, percolating rainwater serves to redistribute this finite source mass throughout the full thickness of the surface soil column.

Biodegradation during leaching to groundwater. By activating this option, it is possible to account for biodegradation during the leaching in the unsaturated zone. In this case the user must define the biodegradation kinetic constant in the screen with the chemical properties of selected contaminants.

GROUNDWATER DISPERSION

Groundwater Dispersion. For the transport of contaminants in groundwater the user can select the type of equation to be used as a function of the expected dispersion. In particular, it is possible to simulate the dispersion of contaminants as:

- DAF1 = dispersion in all directions (x, y, z);
- DAF2 = in this case it is assumed that there is transversal and longitudinal dispersion in all directions while the vertical dispersion is assumed to take place only downwards;
- DAF3 = in this case it is assumed that there is only longitudinal and transversal dispersion (i.e. no vertical dispersion).

The implemented equations are reported in the appendix.

Check on the groundwater mixing zone height. By activating this option, the software automatically uses the DAF3 in the case that the calculated thickness of the mixing zone coincides with the thickness of the aquifer.

Biodegradation during groundwater transport. By activating this option, it is possible to account for biodegradation during the transport of contaminants in groundwater. In this case the user must define the biodegradation kinetic constant in the screen with the chemical properties of selected contaminants.

CSAT

Saturation Concentration (Csat). If this option is activated by the user, the software calculates the saturation concentration in the soil (Csat) at which the contaminant reaches the solubility value in the dissolved phase and the vapor pressure in the soil-gas. In this case, for the indirect exposure pathways (volatilization and leaching) for saturation conditions (i.e. CRS> Csat) the risks are calculated assuming as the solubility value in the dissolved phase and the vapor pressure in the soil-gas. For the direct exposure pathways (i.e. soil ingestion and dermal contact) these concentrations, although higher the saturation concentration does not affect the estimation of the risks as the receptor might be exposed also to the separate phase. With regard to the calculation of the clean-up levels, if the calculated SSTL are higher than the Csat value in the output screen these values are not shown but it is indicated that the SSTL are higher than Csat (indicated as '> Csat'). Indeed, the achievement of SSTL > Csat indicates for the indirect exposure pathways (volatilization and leaching) even at the maximum concentration at which the contaminant can leach (solubility) or volatilize (vapor pressure) the risks are below the acceptable levels (e.g. $R = 10^{-6}$ or HI = 1). In the event that the Csat option is deselected, a sub-option can be activated in which the Csat is verified only in the calculation of the

SSTL but not in the direct calculation of the Risk (i.e. the CRS is not limited to the Csat). This sub-option, although can lead to inconsistent results in the two calculation modes (Risk Calculation and Calculation of SSTL), has been planned to replicate the results of other available software (e.g. RBCA ToolKit) that only perform the verification of the Csat in the calculation of the SSTL but not in the calculation of the Risk.

Source depletion. By activating this option, in the mass balance used for the estimation of the source depletion the software accounts for the presence (if any) of separate phase in the subsurface.

EXPOSURE

Adjustement factor for carcinogenic parameters of children (ADAF). By activating this option, the software applies an adjustment factor (ADAF) to the toxicological parameters (carcinogenic effects) used for the estimation of risks and clean-up levels in the case of children as receptors. The values of ADAF used by the software can be modified in the screen with the definition of the toxicological parameters for the selected contaminants.

RfD vs RfC. For the inhalation pathway, the user can select the method to be used for the estimation of the risks and of the clean-up levels. The software employs two methods. The first is based on the use of a reference dose (RfD and SF) and the risks are calculated as a function of the body weight and of the inhalation rate. The second method is based on the use of a reference concentration without any adjustment for the body weight or the inhalation rate.

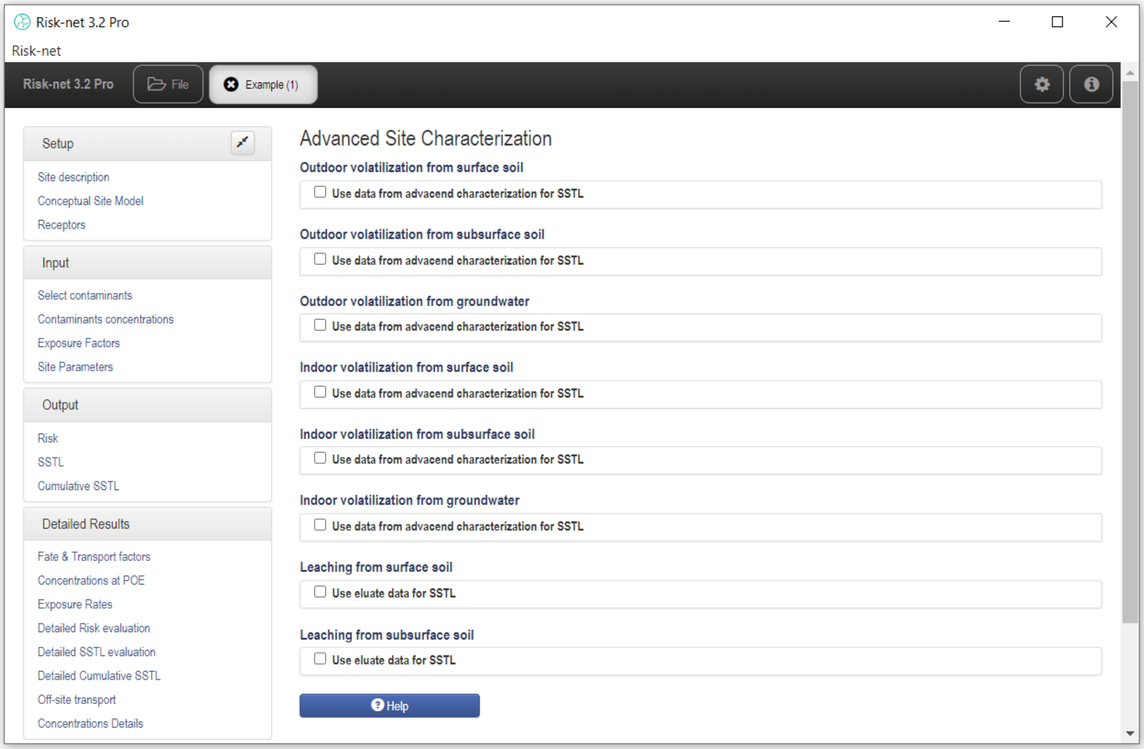
Bioaccessibility. For the soil ingestion pathway, by activating this option, the software accounts in the estimation of risks and SSTLs for the bioaccessibile fraction. The bioaccessible fraction can be defined in the screen that reports the chemico-physical properties of the contaminants of concern

LIMITS

Limits. Here the user can set the acceptable individual (single contaminant) and cumulative (multiple contaminants) acceptable risk (carcinogenic effects) and hazard index (non-carcinogenic effects).

ADVANCED SITE CHARACTERIZATION

This screen (Figure 16) is accessed by clicking "Advanced Characterization" on the "Advanced Options" menu.



Advanced Site Characterization

Outdoor volatilization from surface soil
☐ Use data from advacend characterization for SSTL

Outdoor volatilization from subsurface soil
☐ Use data from advacend characterization for SSTL

Outdoor volatilization from groundwater
☐ Use data from advacend characterization for SSTL

Indoor volatilization from surface soil
☐ Use data from advacend characterization for SSTL

Indoor volatilization from subsurface soil
☐ Use data from advacend characterization for SSTL

Indoor volatilization from groundwater
☐ Use data from advacend characterization for SSTL

Leaching from surface soil
☐ Use eluate data for SSTL

Leaching from subsurface soil
☐ Use eluate data for SSTL

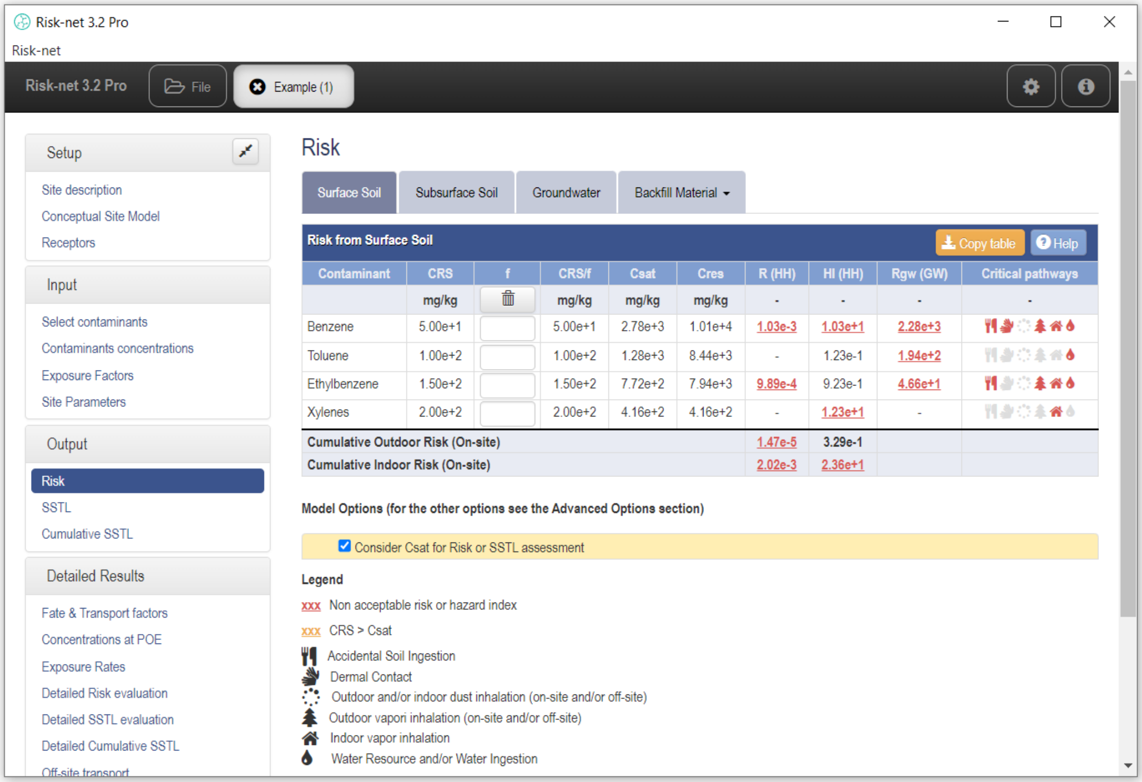
Figure 20. Advanced Site Characterization.

By default, the results from the advanced characterization of the site are only used to estimate the risks for human health and environment for the selected receptor. In this screen the user can decide if these data must be used also for the estimation of the clean-up levels in the surface soil, subsurface soil and in groundwater. In this case, these data are used to calculate a semi-empirical fate and transport factor that is used for the update of the clean-up levels calculated based only on mathematical modelling. For more details, readers are directed to the appendix with the description of the equations implemented in the software.

OUTPUT

RISK

This screen (Figure 21) is accessed by clicking "Risk" on the "Output" menu.



Risk from Surface Soil

Contaminant	CRS	f	CRS/f	Csat	Cres	R (HH)	HI (HH)	Rgw (GW)	Critical pathways
	mg/kg		mg/kg	mg/kg	mg/kg	-	-	-	-
Benzene	5.00e+1		5.00e+1	2.78e+3	1.01e+4	1.03e-3	1.03e+1	2.28e+3	
Toluene	1.00e+2		1.00e+2	1.28e+3	8.44e+3	-	1.23e-1	1.94e+2	
Ethylbenzene	1.50e+2		1.50e+2	7.72e+2	7.94e+3	9.89e-4	9.23e-1	4.66e+1	
Xylenes	2.00e+2		2.00e+2	4.16e+2	4.16e+2	-	1.23e+1	-	
Cumulative Outdoor Risk (On-site)						1.47e-5	3.29e-1		
Cumulative Indoor Risk (On-site)						2.02e-3	2.36e+1		

Model Options (for the other options see the Advanced Options section)

☑ Consider Csat for Risk or SSTL assessment

Legend

xxx Non acceptable risk or hazard index

xxx CRS > Csat

Accidental Soil Ingestion

Dermal Contact

Outdoor and/or indoor dust inhalation (on-site and/or off-site)

Outdoor vapori inhalation (on-site and/or off-site)

Indoor vapor inhalation

Water Resource and/or Water Ingestion

Figure 21. Baseline Risks.

This screen shows the risks for human health (R and HI) individual (for the single contaminant) and cumulative (total, calculated as the sum of the risks of each selected contaminant) and the risks for the groundwater resources (Rgw) calculated for each source selected in the conceptual site model. In red are highlighted the risks higher than the acceptable limits. Furthermore, in the last column of the table, the critical exposure/transport pathways (risks above acceptable limits) are highlighted in red for each contaminant. In yellow are highlighted the source concentrations that are higher than the saturation concentration (or the solubility for the contamination in groundwater). On this screen the user can calculate, iteratively, the concentration in the source that ensures acceptable risks by entering a correction factor for each contaminant in the column 'f'. The "Copy table" command allows the user to copy and paste in Word or Excel the output table (maintaining the table formatting). The contaminants for which the chemico-physical and/or toxicological properties have been modified, are underlined and in italic.

Table 6 describes the different keywords and symbols related to the calculation of the Risk.

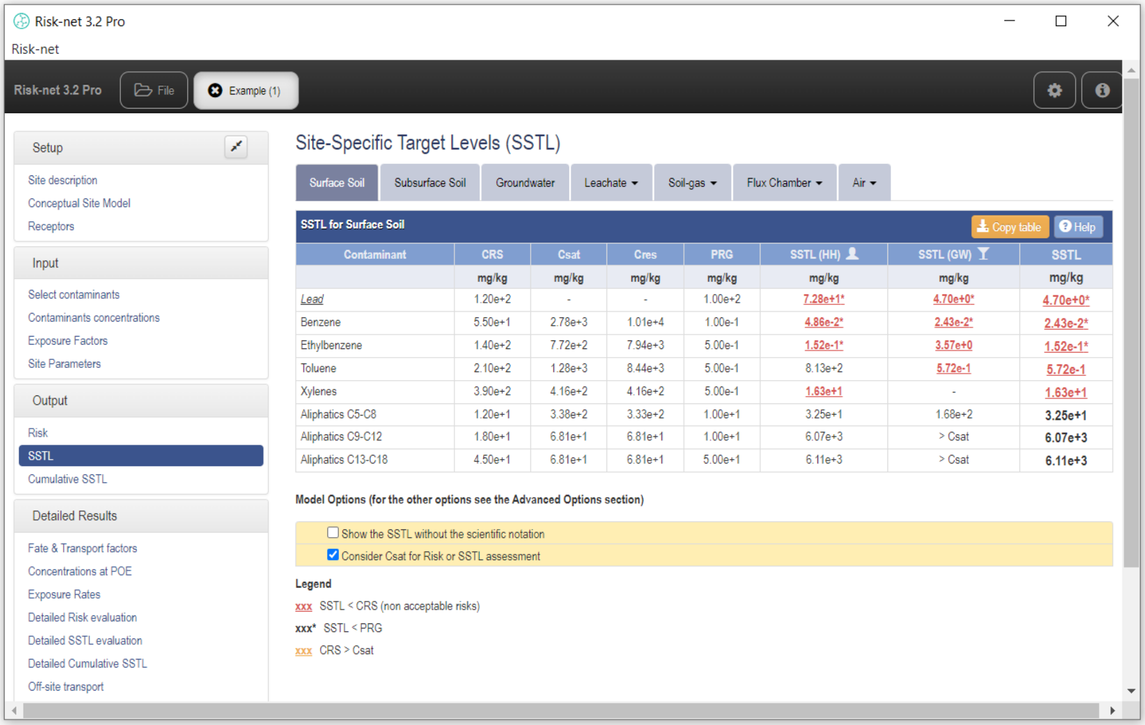
Table 6. Nomenclature in the 'Risk' screen.

SYMBOL	**DEFINITION**
CRS	Source Concentration
f	Reduction factor for CRS
R (HH)	Carcinogenic Risk (human health)
HI	Hazard Index, non-carcinogenic (human health)
Rgw	Risk for the groundwater resource
Csat	Saturation concentration
Cres	Residual Concentration (screening NAPL)
Sol	Solubility

SITE-SPECIFIC TARGET LEVELS (SSTL)

This screen (Figure 22) is accessed by clicking "SSTL" on the "Output" menu.

This screen shows the maximum acceptable concentration in the affected source medium (i.e. the Site-Specific Target Levels, SSTL) for each contaminant of concern that ensures acceptable individual risks for human health (R and HI) and for the groundwater resources (Rgw). In red are highlighted the contaminant for which the source concentration is higher than the calculated SSTL. With an asterisk are highlighted the SSTL that are lower than the PRG (Preliminary Remediation Goals) values defined in the database. In yellow are highlighted the source concentrations that are higher than the saturation concentration (or the solubility for the contamination in groundwater). The "Copy table" command allows the user to copy and paste in Word or Excel the output table (maintaining the table formatting). The contaminants for which the chemico-physical and/or toxicological properties have been modified, are underlined and in italic.



Site-Specific Target Levels (SSTL)

SSTL for Surface Soil

Contaminant	CRS	Csat	Cres	PRG	SSTL (HH)	SSTL (GW)	SSTL
	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg
Lead	1.20e+2	-	-	1.00e+2	7.28e+1*	4.70e+0*	**4.70e+0***
Benzene	5.50e+1	2.78e+3	1.01e+4	1.00e-1	4.86e-2*	2.43e-2*	**2.43e-2***
Ethylbenzene	1.40e+2	7.72e+2	7.94e+3	5.00e-1	1.52e-1*	3.57e+0	**1.52e-1***
Toluene	2.10e+2	1.28e+3	8.44e+3	5.00e-1	8.13e+2	5.72e-1	**5.72e-1**
Xylenes	3.90e+2	4.16e+2	4.16e+2	5.00e-1	1.63e+1	-	**1.63e+1**
Aliphatics C5-C8	1.20e+1	3.38e+2	3.33e+2	1.00e+1	3.25e+1	1.68e+2	**3.25e+1**
Aliphatics C9-C12	1.80e+1	6.81e+1	6.81e+1	1.00e+1	6.07e+3	> Csat	**6.07e+3**
Aliphatics C13-C18	4.50e+1	6.81e+1	6.81e+1	5.00e+1	6.11e+3	> Csat	**6.11e+3**

Model Options (for the other options see the Advanced Options section)

☐ Show the SSTL without the scientific notation
☑ Consider Csat for Risk or SSTL assessment

Legend

xxx SSTL < CRS (non acceptable risks)
xxx* SSTL < PRG
xxx CRS > Csat

Figure 22. Site-Specific Target Levels (SSTL).

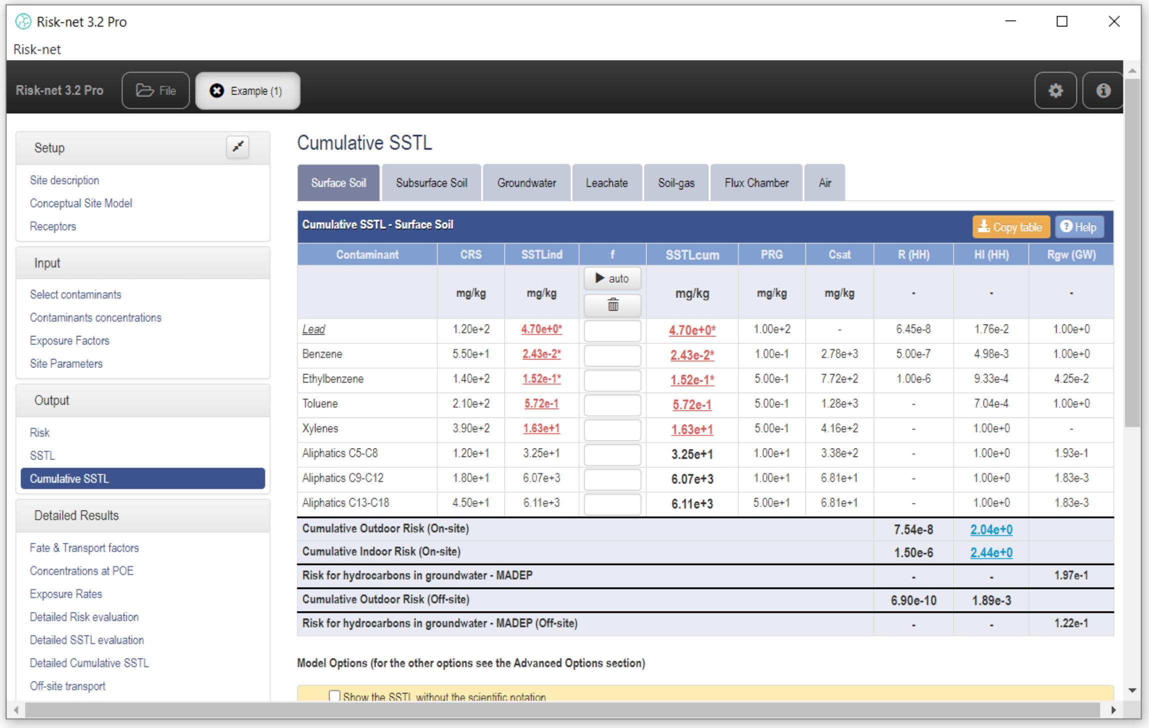
Table 7 describes the different keywords and symbols related to the calculation of the SSTLs.

Table 7. Nomenclature in the ‘SSTL’ screen.

SYMBOL	DEFINITION
CRS	Source Concentration
SSTL (HH)	Site-Specific Target Levels for human health
SSTL (GW)	Site-Specific Target Levels for the groundwater resource
Csat	Saturation concentration
Cres	Residual Concentration (screening NAPL)
Sol	Solubility
PRG	Preliminary Remediation Goals

CUMULATIVE SSTL

This screen (Figure 23) is accessed by clicking "Cumulative SSTL" on the "Output" menu.



Cumulative SSTL - Surface Soil

Contaminant	CRS	SSTLind	f	SSTLcum	PRG	Csat	R (HH)	HI (HH)	Rgw (GW)
	mg/kg	mg/kg		mg/kg	mg/kg	mg/kg	-	-	-
Lead	1.20e+2	4.70e+0*		4.70e+0*	1.00e+2	-	6.45e-8	1.76e-2	1.00e+0
Benzene	5.50e+1	2.43e-2*		2.43e-2*	1.00e-1	2.78e+3	5.00e-7	4.98e-3	1.00e+0
Ethylbenzene	1.40e+2	1.52e-1*		1.52e-1*	5.00e-1	7.72e+2	1.00e-6	9.33e-4	4.25e-2
Toluene	2.10e+2	5.72e-1		5.72e-1	5.00e-1	1.28e+3	-	7.04e-4	1.00e+0
Xylenes	3.90e+2	1.63e+1		1.63e+1	5.00e-1	4.16e+2	-	1.00e+0	-
Aliphatics C5-C8	1.20e+1	3.25e+1		**3.25e+1**	1.00e+1	3.38e+2	-	1.00e+0	1.93e-1
Aliphatics C9-C12	1.80e+1	6.07e+3		**6.07e+3**	1.00e+1	6.81e+1	-	1.00e+0	1.83e-3
Aliphatics C13-C18	4.50e+1	6.11e+3		**6.11e+3**	5.00e+1	6.81e+1	-	1.00e+0	1.83e-3
Cumulative Outdoor Risk (On-site)							**7.54e-8**	2.04e+0	
Cumulative Indoor Risk (On-site)							**1.50e-6**	2.44e+0	
Risk for hydrocarbons in groundwater - MADEP							-	-	**1.97e-1**
Cumulative Outdoor Risk (Off-site)							**6.90e-10**	**1.89e-3**	
Risk for hydrocarbons in groundwater - MADEP (Off-site)							-	-	**1.22e-1**

Model Options (for the other options see the Advanced Options section)

☐ Show the SSTL without the scientific notation

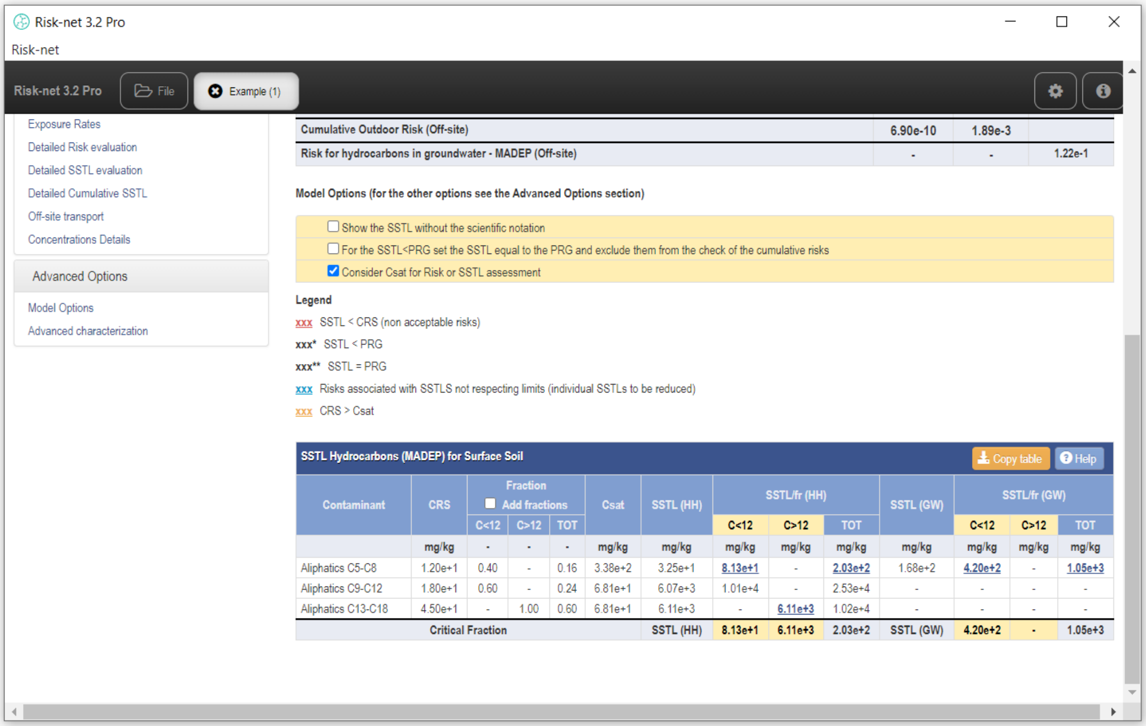
Figure 23. Cumulative Site-Specific Target Levels (SSTL).

From this screen the user can check whether the individual SSTL (SSTLind) calculated for each contaminant ensures acceptable cumulative risks (related to the simultaneous presence of several substances). If the cumulative risks are not acceptable (cells in blue) the user should reduce SSTLind until to find a SSTL that ensures the respect of both the individual and cumulative risks. This can be done by iteratively operating on the adjustment factor in the column 'f' column until to get acceptable cumulative risks. The button 'auto' in the column 'f' automatically insert a correction factor equal to the number of contaminants selected (very conservative option). The reduced SSTL (SSTL / f), that ensures the respect of both the individual and cumulative risks, represents the cumulative SSTL (SSTL cum). The contaminants for which the chemico-physical and/or toxicological properties have been modified, are underlined and in italic.
Table 8 describes the different keywords and symbols related to the calculation of the Cumulative SSTLs.

Table 8. Nomenclature in the ‘Cumulative SSTL’ screen.

SYMBOL	DEFINITION
CRS	Source Concentration
f	Reduction factor for SSTL
R (HH)	Carcinogenic Risk (human health)
HI	Hazard Index, non-carcinogenic (human health)
Rgw	Risk for the groundwater resource
Csat	Saturation concentration
Cres	Residual Concentration (screening NAPL)
Sol	Solubility
SSTLind	Individual Site-Specific Target Levels
SSTLcum	Cumulative Site-Specific Target Levels (SSTLind/f)
PRG	Preliminary Remediation Goals

SSTLs Hydrocarbons. If in the contaminants of concern the user select hydrocarbons compounds classified as MADEP or TPH WG, in the Cumulative SSTL screen the user can find a further table with the SSTLs calculated for "Hydrocarbons C>12" and "Hydrocarbons C<12" and "Total hydrocarbons". This screen shows the SSTL for Light (C <12), Heavy (C> 12) and Total Hydrocarbons (TOT) calculated with the ‘critical fraction’ method based on the different hydrocarbon’s classes selected by the user. Specifically, the calculation is performed for both MADEP and TPHCWG speciation. The most critical class is identified as a function of the SSTL calculated for each class and the fraction of the class presents in the mixture (estimated on the basis of the concentration set by the user). For more details, readers are directed to the appendix with the description of the equations implemented in the software.



Cumulative Outdoor Risk (Off-site)	**6.90e-10**	**1.89e-3**	
Risk for hydrocarbons in groundwater - MADEP (Off-site)	**-**	**-**	**1.22e-1**

Model Options (for the other options see the Advanced Options section)

☐ Show the SSTL without the scientific notation
☐ For the SSTL<PRG set the SSTL equal to the PRG and exclude them from the check of the cumulative risks
☑ Consider Csat for Risk or SSTL assessment

Legend

xxx SSTL < CRS (non acceptable risks)
xxx* SSTL < PRG
xxx** SSTL = PRG
xxx Risks associated with SSTLS not respecting limits (individual SSTLs to be reduced)
xxx CRS > Csat

SSTL Hydrocarbons (MADEP) for Surface Soil

Contaminant	CRS	Fraction ☐ Add fractions			Csat	SSTL (HH)	SSTL/fr (HH)			SSTL (GW)	SSTL/fr (GW)		
		C<12	C>12	TOT			C<12	C>12	TOT		C<12	C>12	TOT
	mg/kg	-	-	-	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg
Aliphatics C5-C8	1.20e+1	0.40	-	0.16	3.38e+2	3.25e+1	8.13e+1	-	2.03e+2	1.68e+2	4.20e+2	-	1.05e+3
Aliphatics C9-C12	1.80e+1	0.60	-	0.24	6.81e+1	6.07e+3	1.01e+4	-	2.53e+4	-	-	-	-
Aliphatics C13-C18	4.50e+1	-	1.00	0.60	6.81e+1	6.11e+3	-	6.11e+3	1.02e+4	-	-	-	-
Critical Fraction						**SSTL (HH)**	**8.13e+1**	**6.11e+3**	**2.03e+2**	**SSTL (GW)**	**4.20e+2**	**-**	**1.05e+3**

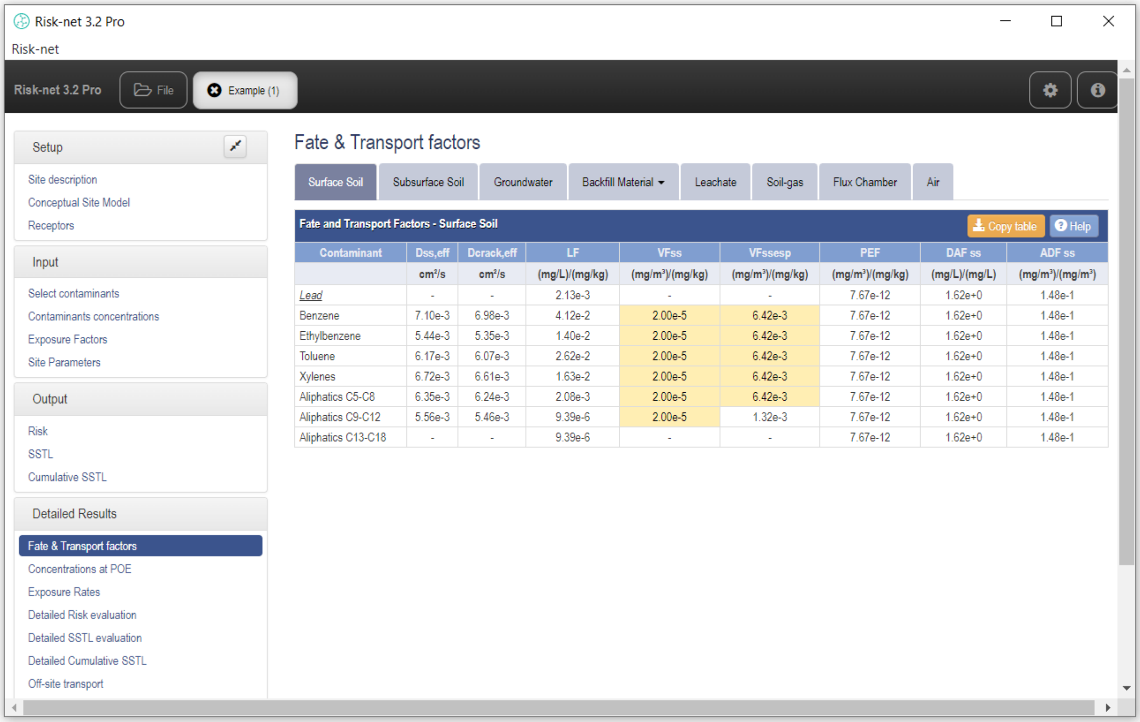
Figure 24. SSTL for TPH mixtures.

DETAILED RESULTS

In addition to the main outputs described in the previous paragraphs, the user can verify in detail the results obtained in the different calculation steps as briefly described below.

FATE & TRANSPORT FACTORS

This screen shows the fate & transport factors (FT) calculated for the migration pathways activated in the conceptual site model. In yellow are highlighted the FT equal to the mass balance in the source (if this option has been activated in the 'model options' screen). In purple are highlighted the semi-empirical FT that were calculated based on the available advanced characterization data (if this option has been activated in the 'advanced characterization' screen). The contaminants for which the chemico-physical and/or toxicological properties have been modified, are underlined and in italic.



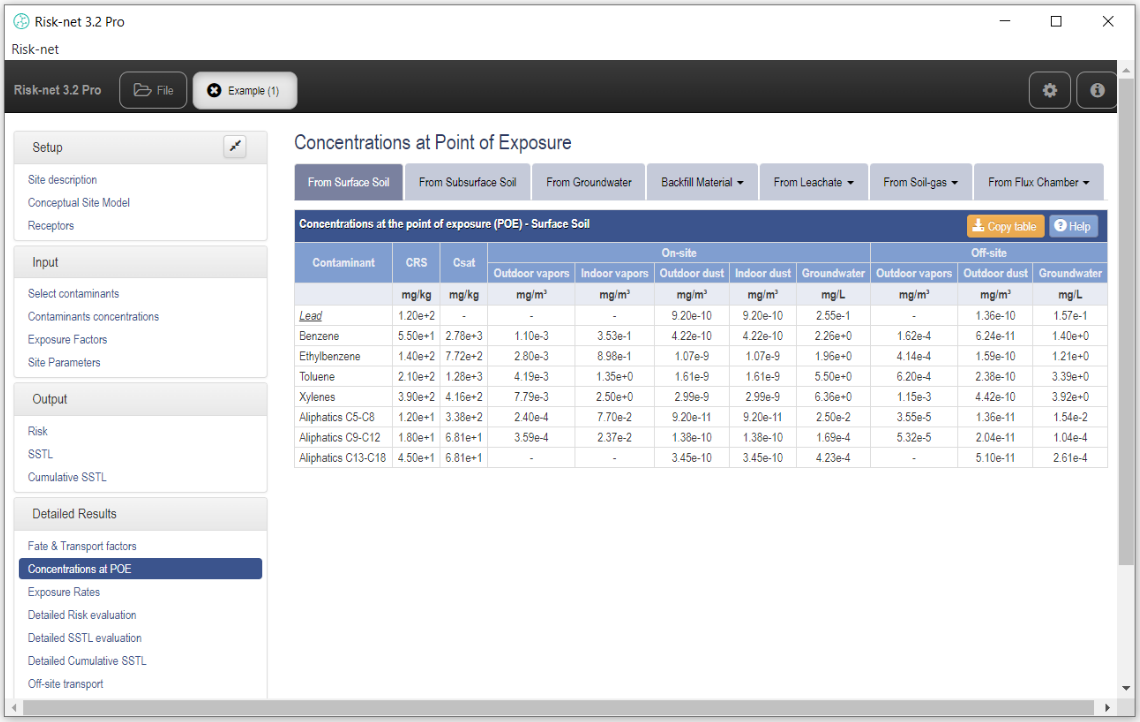
Fate and Transport Factors - Surface Soil

Contaminant	Dss,eff	Dcrack,eff	LF	VFss	VFssesp	PEF	DAF ss	ADF ss
	cm^2/s	cm^2/s	(mg/L)/(mg/kg)	$(mg/m^3)/(mg/kg)$	$(mg/m^3)/(mg/kg)$	$(mg/m^3)/(mg/kg)$	(mg/L)/(mg/L)	$(mg/m^3)/(mg/m^3)$
Lead	-	-	2.13e-3	-	-	7.67e-12	1.62e+0	1.48e-1
Benzene	7.10e-3	6.98e-3	4.12e-2	2.00e-5	6.42e-3	7.67e-12	1.62e+0	1.48e-1
Ethylbenzene	5.44e-3	5.35e-3	1.40e-2	2.00e-5	6.42e-3	7.67e-12	1.62e+0	1.48e-1
Toluene	6.17e-3	6.07e-3	2.62e-2	2.00e-5	6.42e-3	7.67e-12	1.62e+0	1.48e-1
Xylenes	6.72e-3	6.61e-3	1.63e-2	2.00e-5	6.42e-3	7.67e-12	1.62e+0	1.48e-1
Aliphatics C5-C8	6.35e-3	6.24e-3	2.08e-3	2.00e-5	6.42e-3	7.67e-12	1.62e+0	1.48e-1
Aliphatics C9-C12	5.56e-3	5.46e-3	9.39e-6	2.00e-5	1.32e-3	7.67e-12	1.62e+0	1.48e-1
Aliphatics C13-C18	-	-	9.39e-6	-	-	7.67e-12	1.62e+0	1.48e-1

Figure 25. Fate & Transport Factors.

CONCENTRATIONS AT THE POINT OF EXPOSURE

This screen shows the concentration at the point of exposure calculated with the fate & transport factors based on the source concentration set by the user for the different migration pathways activated in the conceptual site model. The contaminants for which the chemico-physical and/or toxicological properties have been modified, are underlined and in italic.



Concentrations at Point of Exposure

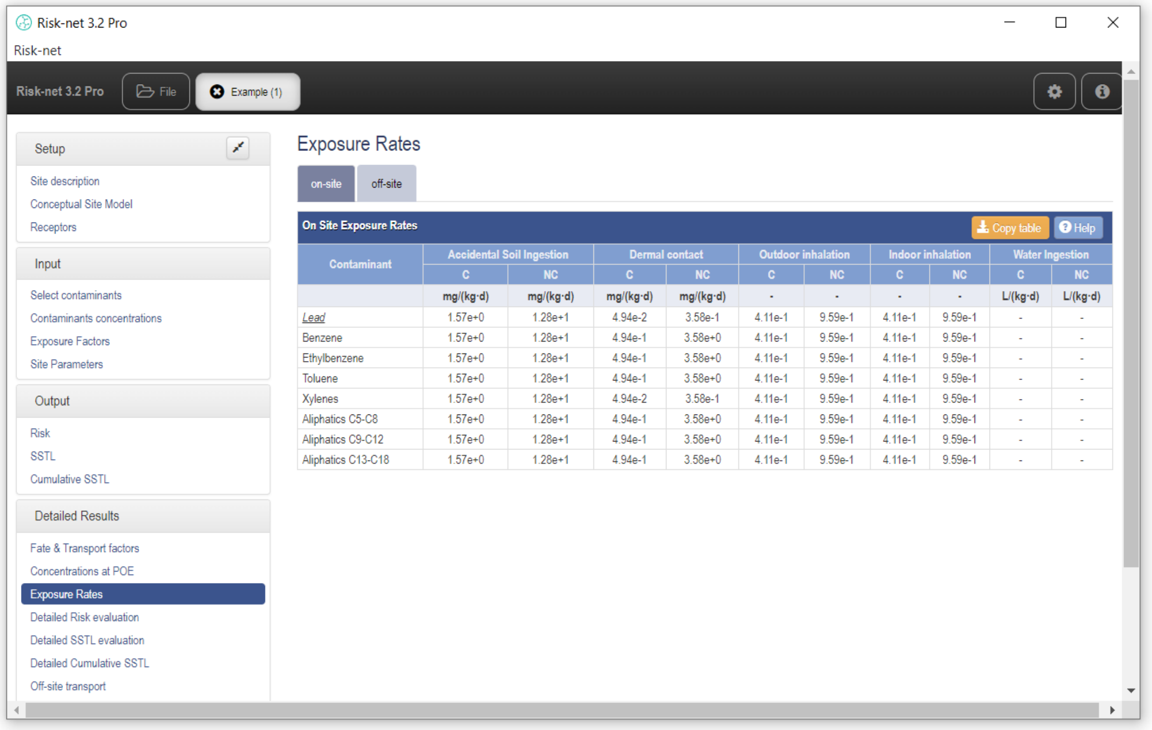
Concentrations at the point of exposure (POE) - Surface Soil

Contaminant	CRS	Csat	On-site					Off-site		
			Outdoor vapors	Indoor vapors	Outdoor dust	Indoor dust	Groundwater	Outdoor vapors	Outdoor dust	Groundwater
	mg/kg	mg/kg	mg/m³	mg/m³	mg/m³	mg/m³	mg/L	mg/m³	mg/m³	mg/L
<u>Lead</u>	1.20e+2	-	-	-	9.20e-10	9.20e-10	2.55e-1	-	1.36e-10	1.57e-1
Benzene	5.50e+1	2.78e+3	1.10e-3	3.53e-1	4.22e-10	4.22e-10	2.26e+0	1.62e-4	6.24e-11	1.40e+0
Ethylbenzene	1.40e+2	7.72e+2	2.80e-3	8.98e-1	1.07e-9	1.07e-9	1.96e+0	4.14e-4	1.59e-10	1.21e+0
Toluene	2.10e+2	1.28e+3	4.19e-3	1.35e+0	1.61e-9	1.61e-9	5.50e+0	6.20e-4	2.38e-10	3.39e+0
Xylenes	3.90e+2	4.16e+2	7.79e-3	2.50e+0	2.99e-9	2.99e-9	6.36e+0	1.15e-3	4.42e-10	3.92e+0
Aliphatics C5-C8	1.20e+1	3.38e+2	2.40e-4	7.70e-2	9.20e-11	9.20e-11	2.50e-2	3.55e-5	1.36e-11	1.54e-2
Aliphatics C9-C12	1.80e+1	6.81e+1	3.59e-4	2.37e-2	1.38e-10	1.38e-10	1.69e-4	5.32e-5	2.04e-11	1.04e-4
Aliphatics C13-C18	4.50e+1	6.81e+1	-	-	3.45e-10	3.45e-10	4.23e-4	-	5.10e-11	2.61e-4

Figure 26. Concentration at the point of exposure.

EXPOSURE RATES

This screen reports the intake rates calculated for the different exposure pathways for each receptor activated by the user. The contaminants for which the chemico-physical and/or toxicological properties have been modified, are underlined and in italic.



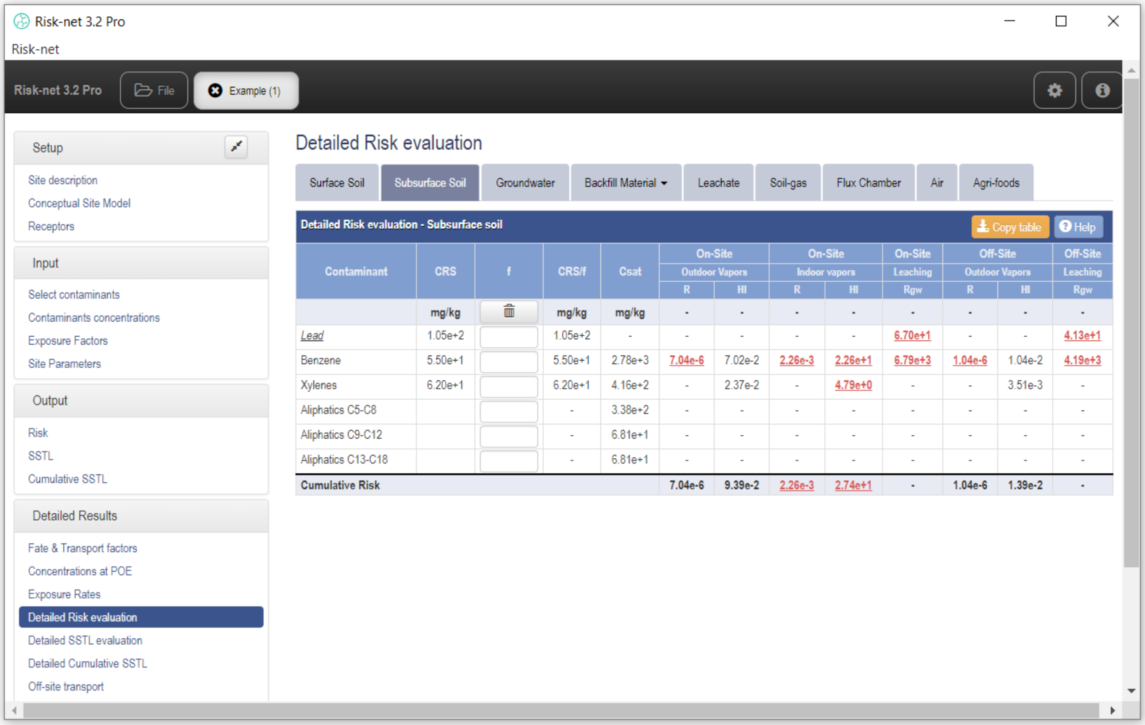
On Site Exposure Rates

Contaminant	Accidental Soil Ingestion		Dermal contact		Outdoor inhalation		Indoor inhalation		Water Ingestion	
	C	NC	C	NC	C	NC	C	NC	C	NC
	mg/(kg·d)	mg/(kg·d)	mg/(kg·d)	mg/(kg·d)	-	-	-	-	L/(kg·d)	L/(kg·d)
Lead	1.57e+0	1.28e+1	4.94e-2	3.58e-1	4.11e-1	9.59e-1	4.11e-1	9.59e-1	-	-
Benzene	1.57e+0	1.28e+1	4.94e-1	3.58e+0	4.11e-1	9.59e-1	4.11e-1	9.59e-1	-	-
Ethylbenzene	1.57e+0	1.28e+1	4.94e-1	3.58e+0	4.11e-1	9.59e-1	4.11e-1	9.59e-1	-	-
Toluene	1.57e+0	1.28e+1	4.94e-1	3.58e+0	4.11e-1	9.59e-1	4.11e-1	9.59e-1	-	-
Xylenes	1.57e+0	1.28e+1	4.94e-2	3.58e-1	4.11e-1	9.59e-1	4.11e-1	9.59e-1	-	-
Aliphatics C5-C8	1.57e+0	1.28e+1	4.94e-1	3.58e+0	4.11e-1	9.59e-1	4.11e-1	9.59e-1	-	-
Aliphatics C9-C12	1.57e+0	1.28e+1	4.94e-1	3.58e+0	4.11e-1	9.59e-1	4.11e-1	9.59e-1	-	-
Aliphatics C13-C18	1.57e+0	1.28e+1	4.94e-1	3.58e+0	4.11e-1	9.59e-1	4.11e-1	9.59e-1	-	-

Figure 27. Exposure Rates.

DETAILED RISK EVALUATION

This screen shows the risks for human health (R and HI) individual (for the single contaminant) and cumulative (total, calculated as the sum of the risks of each selected contaminant) and the risks for the groundwater resources (RGW) calculated for each source selected in the conceptual site model. In red are highlighted the risks higher than the acceptable limits. In yellow are highlighted the source concentrations that are higher than the saturation concentration (or the solubility for the contamination in groundwater). On this screen the user can calculate, iteratively, the concentration in the source that ensures acceptable risks by entering a correction factor for each contaminant in the column 'f'. The contaminants for which the chemico-physical and/or toxicological properties have been modified, are underlined and in italic.



Detailed Risk evaluation

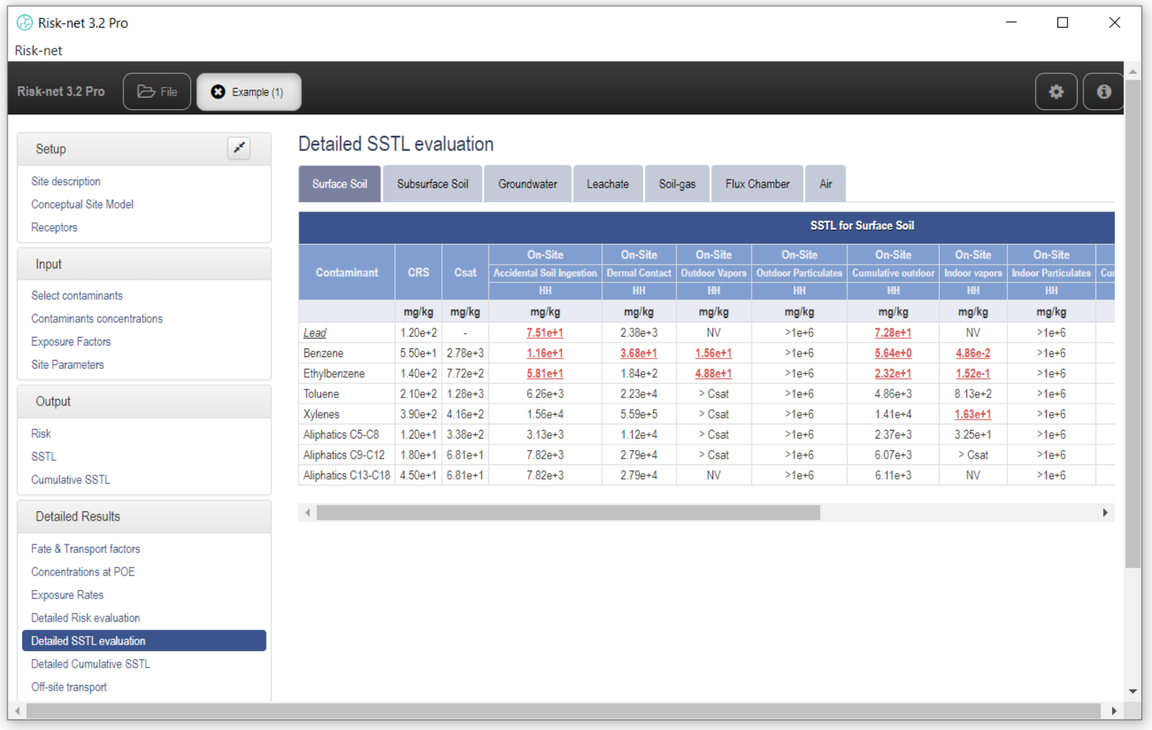
Detailed Risk evaluation - Subsurface soil

Contaminant	CRS	f	CRS/f	Csat	On-Site Outdoor Vapors		On-Site Indoor vapors		On-Site Leaching	Off-Site Outdoor Vapors		Off-Site Leaching
					R	HI	R	HI	Rgw	R	HI	Rgw
	mg/kg		mg/kg	mg/kg	-	-	-	-	-	-	-	-
Lead	1.05e+2		1.05e+2	-	-	-	-	-	6.70e+1	-	-	4.13e+1
Benzene	5.50e+1		5.50e+1	2.78e+3	7.04e-6	7.02e-2	2.26e-3	2.26e+1	6.79e+3	1.04e-6	1.04e-2	4.19e+3
Xylenes	6.20e+1		6.20e+1	4.16e+2	-	2.37e-2	-	4.79e+0	-	-	3.51e-3	-
Aliphatics C5-C8			-	3.38e+2	-	-	-	-	-	-	-	-
Aliphatics C9-C12			-	6.81e+1	-	-	-	-	-	-	-	-
Aliphatics C13-C18			-	6.81e+1	-	-	-	-	-	-	-	-
Cumulative Risk					**7.04e-6**	**9.39e-2**	2.26e-3	2.74e+1	**-**	**1.04e-6**	**1.39e-2**	**-**

Figure 28. Detailed Risk Evaluation.

DETAILED SSTL EVALUATION

This screen shows the maximum acceptable concentration in the affected source medium (i.e. the Site-Specific Target Levels, SSTL) for each contaminant of concern that ensures acceptable individual risks for human health (R and HI) and for the groundwater resources (Rgw). In red are highlighted the contaminant for which the source concentration is higher than the calculated SSTL. With an asterisk are highlighted the SSTL that are lower than the PRG (Preliminary Remediation Goals) values defined in the database. In yellow are highlighted the source concentrations that are higher than the saturation concentration (or the solubility for the contamination in groundwater). The contaminants for which the chemico-physical and/or toxicological properties have been modified, are underlined and in italic.



Detailed SSTL evaluation

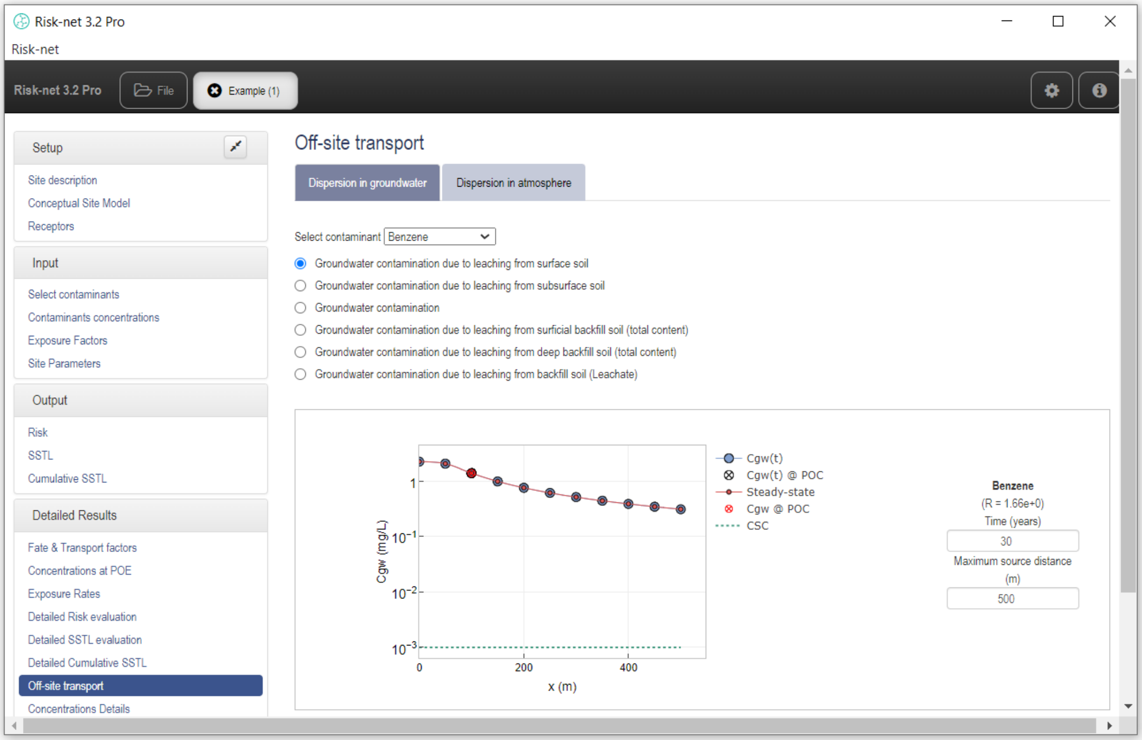
SSTL for Surface Soil

Contaminant	CRS	Csat	On-Site Accidental Soil Ingestion HH	On-Site Dermal Contact HH	On-Site Outdoor Vapors HH	On-Site Outdoor Particulates HH	On-Site Cumulative outdoor HH	On-Site Indoor vapors HH	On-Site Indoor Particulates HH
	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg	mg/kg
Lead	1.20e+2	-	**7.51e+1**	2.38e+3	NV	>1e+6	**7.28e+1**	NV	>1e+6
Benzene	5.50e+1	2.78e+3	**1.16e+1**	**3.68e+1**	**1.56e+1**	>1e+6	**5.64e+0**	**4.86e-2**	>1e+6
Ethylbenzene	1.40e+2	7.72e+2	**5.81e+1**	1.84e+2	**4.88e+1**	>1e+6	**2.32e+1**	**1.52e-1**	>1e+6
Toluene	2.10e+2	1.28e+3	6.26e+3	2.23e+4	> Csat	>1e+6	4.86e+3	8.13e+2	>1e+6
Xylenes	3.90e+2	4.16e+2	1.56e+4	5.59e+5	> Csat	>1e+6	1.41e+4	**1.63e+1**	>1e+6
Aliphatics C5-C8	1.20e+1	3.38e+2	3.13e+3	1.12e+4	> Csat	>1e+6	2.37e+3	3.25e+1	>1e+6
Aliphatics C9-C12	1.80e+1	6.81e+1	7.82e+3	2.79e+4	> Csat	>1e+6	6.07e+3	> Csat	>1e+6
Aliphatics C13-C18	4.50e+1	6.81e+1	7.82e+3	2.79e+4	NV	>1e+6	6.11e+3	NV	>1e+6

Figure 29. Detailed SSTL Evaluation.

OFF-SITE TRANSPORT

This screen can be used to evaluate the off-site transport of contaminants in the groundwater or in the atmosphere. In particular, the user must select from the dropdown menu the contaminant and the matrix of concern. In the case of the transport in groundwater, the graphs show the concentration of the selected contaminant as a function of time and space. In the case of the dispersion of the contaminants in the atmosphere the graphs show only the concentration as a function of the distance from the site. The user can change the distances and the times at which to calculate the concentrations by operating on the boxes reported in the table of interest.



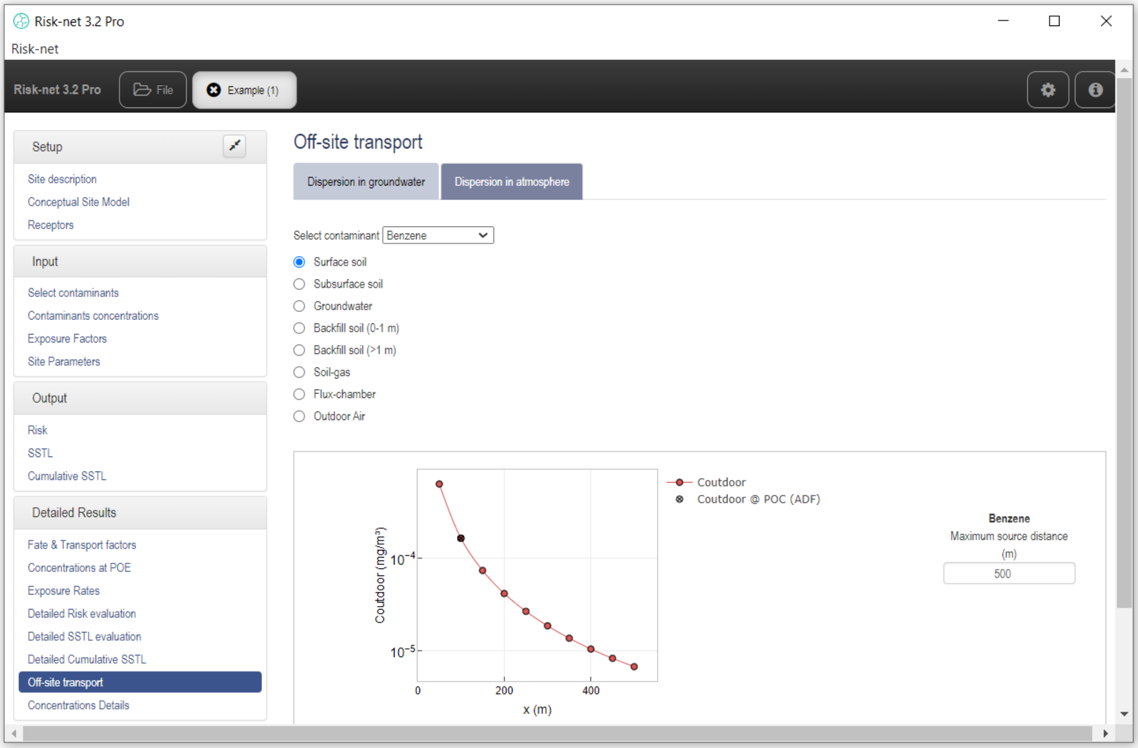
Off-site transport

Select contaminant Benzene

● Groundwater contamination due to leaching from surface soil
○ Groundwater contamination due to leaching from subsurface soil
○ Groundwater contamination
○ Groundwater contamination due to leaching from surficial backfill soil (total content)
○ Groundwater contamination due to leaching from deep backfill soil (total content)
○ Groundwater contamination due to leaching from backfill soil (Leachate)

Benzene
(R = 1.66e+0)
Time (years) 30
Maximum source distance (m) 500

Figure 30. Off-site transport (groundwater).



Off-site transport

Select contaminant Benzene

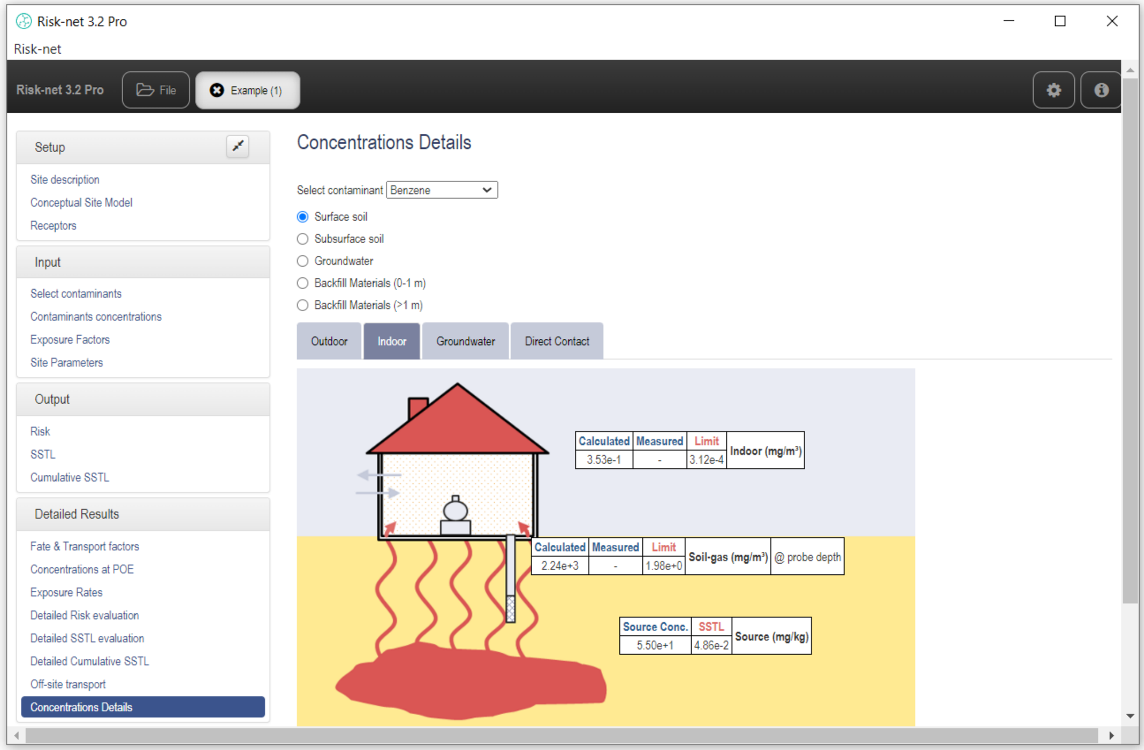
● Surface soil
○ Subsurface soil
○ Groundwater
○ Backfill soil (0-1 m)
○ Backfill soil (>1 m)
○ Soil-gas
○ Flux-chamber
○ Outdoor Air

Benzene
Maximum source distance (m) 500

Figure 31. Off-site transport (atmosphere).

CONCENTRATIONS DETAILS

Here the user must select from the 2 drop-down menu the matrix (surface soil, subsurface soil, groundwater or backfill material) and the contaminant of interest (among those selected by the user as chemical of concern). Based on the matrix and contaminant selected, this screen reports the concentrations expected in different matrices (i.e. soil gas, eluate, outdoor air, indoor air ...) and the corresponding measured value (if available). In practice, this screen can be of help in evaluating the reliability of the screening model to predict the partition and transport of contaminants in the subsurface.



Concentrations Details

Select contaminant Benzene

● Surface soil
○ Subsurface soil
○ Groundwater
○ Backfill Materials (0-1 m)
○ Backfill Materials (>1 m)

Calculated	Measured	Limit	Indoor (mg/m³)
3.53e-1	-	3.12e-4	

Calculated	Measured	Limit	Soil-gas (mg/m³)	@ probe depth
2.24e+3	-	1.98e+0		

Source Conc.	SSTL	Source (mg/kg)
5.50e+1	4.86e-2	

Figure 32. Concentrations Details.

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APPENDICES – EQUATIONS AND MODELING PROCEDURES

APP. 1A. RISK CALCULATION (SOIL AND GROUNDWATER)

Individual Risk. The estimation of risks for human health, correlated to exposure to a contaminant, is calculated in the software by applying the following equations:

$R = E \cdot SF$ Risk for carcinogenic contaminants

$HI = E / RfD$ Hazard Index for non-carcinogenic contaminants

Where *E* is the daily chronic contaminant exposure rate, *SF* the slope factor (i.e. the probability of incremental cancer case occurrence per unit dose) and *RfD* the reference dose (i.e. the daily exposure rate that does not induce adverse effects on humans during the entire life).

The chronic daily contaminant assumption, *E*, is given by multiplying the concentration of the contaminant at the point of exposure, C_{poe}, with the effective exposure rate *EM* (e.g. the daily ingested soil amount or inhaled air volume per unit body weight)

$$E = C_{poe} \cdot EM$$

The concentration at the point of exposure, C_{poe}, may be calculated by applying the following equation:

$$C_{poe} = FT \cdot CRS$$

where *CRS* is the representative source concentration and *FT* the fate and transport factor used for the selected migration pathway.

Combining these equations, the risk and the hazard index can be calculated as follows:

$R = FT \cdot CRS \cdot EM \cdot SF$ Risk for carcinogenic contaminants

$HI = \dfrac{FT \cdot CRS \cdot EM}{RfD}$ Hazard Index for non-carcinogenic contaminants

This calculation is performed for the different exposure and migration pathways active in the site using the appropriate exposure and fate & transport factors (for details, see the tables below). The equations for the calculation of the different fate and transport factors (FT) are reported in Appendix 3. The equations for the calculation of the different intake rates are reported in Appendix 4.

Note that the above equations are those reported in the ISPRA guidelines (2008) that are based on the use of the Reference Dose (RfD) and the Slope Factor (SF). However, for the inhalation pathway the software allows the user to use the approach based on the Reference Concentration (RfC) and the Inhalation Unit Risk (IUR) using the following equations:

$R = FT \cdot CRS \cdot EC \cdot IUR$ Risk for carcinogenic contaminants

$HI = \frac{FT \cdot CRS \cdot EC}{RfC}$ Hazard Index for non-carcinogenic contaminants

In the following tables, the equations implemented in the software are distinguished as “reference dose method” and “reference concentration method”

Multiple exposure pathways. The following report the criteria used in the software for the calculation of the individual risk for each media of concern accounting for multiple exposure pathways.

SURFACE SOIL

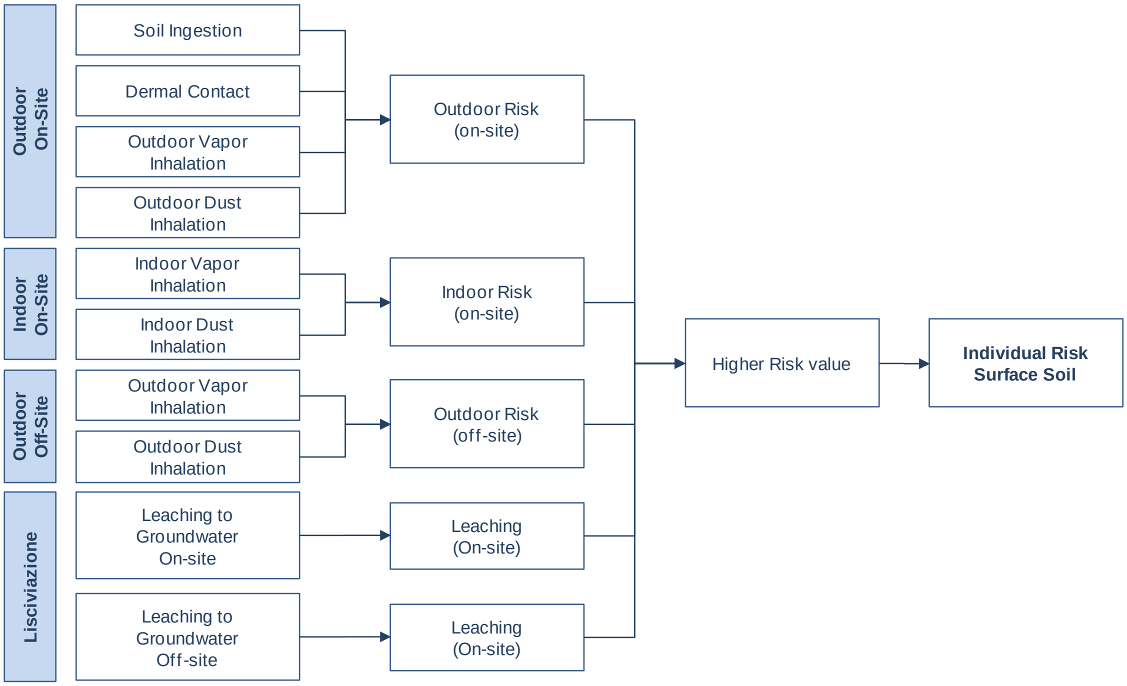

Figure 33. Risk – Surface soil. Multiple exposures.

SUBSURFACE SOIL

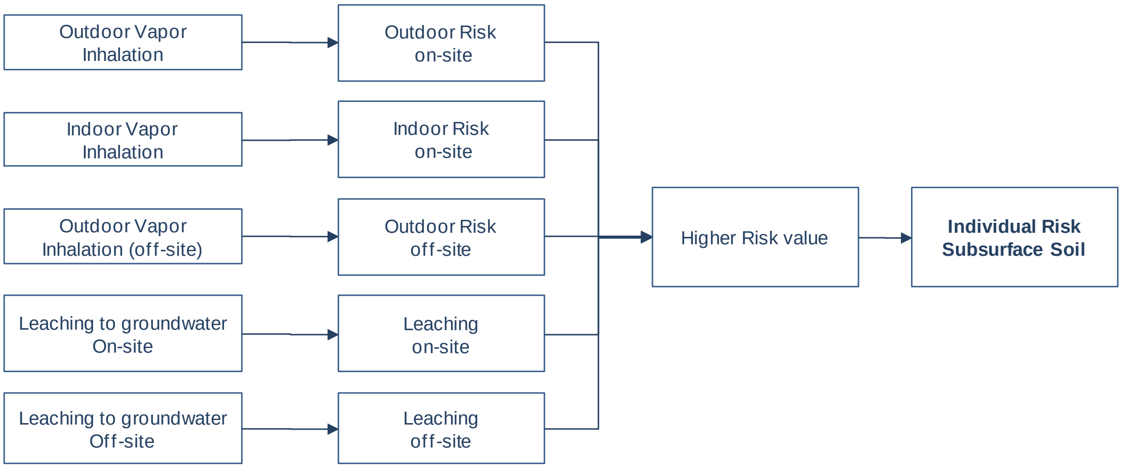

Figure 34. Risk – Subsurface soil. Multiple exposures.

GROUNDWATER

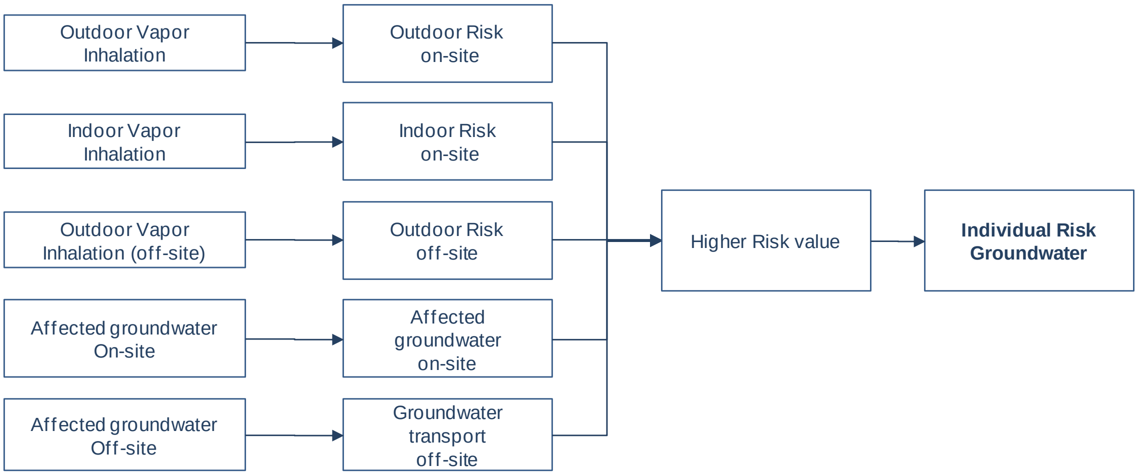

Figure 35. Risk – Groundwater. Multiple exposures.

Cumulative Risk. The cumulative risk is calculated as the sum of the incremental risk (R_i and HI_i) values associated to each contaminant of concern (i) as follows:

$$R_{tot} = \sum_{i=1}^{n} R_i$$

Cumulative risk for carcinogenic contaminants

$HI_{tot} = \sum_{i=1}^{n} HI_i$ Cumulative hazard index for non carcinogenic contaminants

Risk for the groundwater resource. The risk for the groundwater resource (R_{GW}) is calculated by comparing the value of concentration of the contaminant in the water table, at the point of compliance (POC) with the reference values defined for the groundwater protection (MCL):

$$R_{GW} = \frac{C_{poe}}{MCL_{GW}} = \frac{FT \cdot CRS}{MCL_{GW}}$$

Table 9. Surface Soil: Risk and Hazard Index

Soil Ingestion (no off-site)

$$R_{SS.IngS} = CRS \cdot SF_{Ing} \cdot EM_{IngS} \cdot 10^{-6}\ kg/mg$$

$$HI_{SS.IngS} = CRS \cdot \frac{EM_{IngS} \cdot 10^{-6}\ kg/mg}{RfD_{Ing}}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
SFI_{ng} = Slope factor - ingestion
RfD I_{ng} = Reference dose - ingestion
EMI_{ngs} = Soil Ingestion rate

Dermal Contact (no off-site)

$$R_{SS.ConD} = CRS \cdot SF_{Ing} \cdot EM_{ConD} \cdot 10^{-6}\ kg/mg$$

$$HI_{SS.ConD} = CRS \cdot \frac{EM_{ConD} \cdot 10^{-6}\ kg/mg}{RfD_{Ing}}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
SFI_{ng} = Slope factor for ingestion
RfD I_{ng} = Reference dose - ingestion
EM_{ConD} = Dermal contact rate

Outdoor Vapor Inhalation *(reference dose method)*

$$R_{SS.InaO} = CRS \cdot SF_{Ina} \cdot EM_{InaO} \cdot VF_{ss} \cdot ADF$$

$$HI_{SS.InaO} = CRS \cdot \frac{EM_{InaO} \cdot VF_{ss} \cdot ADF}{RfD_{Ina}}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose - inhalation
EM_{InaO} = Outdoor inhalation rate
VF_{ss} = Outdoor volatilization factor
ADF = Atmospheric dispersion factor

Outdoor Vapor Inhalation *(reference concentration method)*

$$R_{SS.InaO} = CRS \cdot IUR_{Ina} \cdot EC_{InaO} \cdot VF_{ss} \cdot ADF$$

$$HI_{SS.InaO} = CRS \cdot \frac{EC_{InaO} \cdot VF_{ss} \cdot ADF}{RfC_{Ina}}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaO} = Outdoor inhalation rate
VF_{ss} = Outdoor volatilization factor
ADF = Atmospheric dispersion factor

Outdoor Dust Inhalation *(reference dose method)*

$$R_{SS.InaOP} = CRS \cdot SF_{Ina} \cdot EM_{InaO} \cdot PEF \cdot ADF$$

$$HI_{SS.InaOP} = CRS \cdot \frac{EM_{InaO} \cdot PEF \cdot ADF}{RfD_{Ina}}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose - inhalation
EM_{InaO} = Outdoor inhalation rate
PEF = Partculate emission factor
ADF = Atmospheric dispersion factor

Outdoor Dust Inhalation *(reference concentration method)*

$$R_{SS.InaOP} = CRS \cdot IUR \cdot EC_{InaO} \cdot PEF \cdot ADF$$

$$HI_{SS.InaOP} = CRS \cdot \frac{EC_{InaO} \cdot PEF \cdot ADF}{RfC}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaO} = Outdoor inhalation rate
PEF = Partculate emission factor
ADF = Atmospheric dispersion factor

Outdoor cumulative risk

$$R_{SS.outdoor} = R_{SS.IngS} + R_{SS.ConD} + R_{SS.InaO} + R_{SS.InaOP}$$

$$HI_{SS.outdoor} = HI_{SS.IngS} + HI_{SS.ConD} + HI_{SS.InaO} + HI_{SS.InaOP}$$

Table 9. Surface Soil: Risk and Hazard Index	
Indoor Vapor Inhalation (no off-site) ***(reference dose method)*** $R_{SS.InaI} = CRS \cdot SF_{Ina} \cdot EM_{InaI} \cdot VF_{ssesp}$ $HI_{SS.InaI} = CRS \cdot \frac{EM_{InaI} \cdot VF_{ssesp}}{RfD_{Ina}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI$_{na}$ = Slope factor - inhalation RfD I$_{na}$ = Reference dose - inhalation EM$_{Inal}$ = Indoor inhalation rate VF$_{sesp}$ = Indoor volatilization factor
Indoor Vapor Inhalation (no off-site) ***(reference concentration method)*** $R_{SS.InaI} = CRS \cdot IUR_{Ina} \cdot EC_{InaI} \cdot VF_{ssesp}$ $HI_{SS.InaI} = CRS \cdot \frac{EC_{InaI} \cdot VF_{ssesp}}{RfC_{Ina}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration IUR$_{Ina}$ = Inhalation Unit Risk RfC$_{Ina}$= Reference concentration EC$_{Inal}$ = Indoor inhalation rate VF$_{sesp}$ = Indoor volatilization factor
Indoor Dust Inhalation (no off-site) ***(reference dose method)*** $R_{SS.InaIP} = CRS \cdot SF_{Ina} \cdot EM_{InaI} \cdot PEF_{in}$ $HI_{SS.InaIP} = CRS \cdot \frac{EM_{InaI} \cdot PEF_{in}}{RfD_{Ina}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI$_{na}$ = Slope factor - inhalation RfD I$_{na}$ = Reference dose - inhalation EM$_{Inal}$ = Indoor inhalation rate PEF$_{in}$ = Particulate indoor emission factor
Indoor Dust Inhalation (no off-site) ***(reference concentration method)*** $R_{SS.InaIP} = CRS \cdot IUR \cdot EC_{InaI} \cdot PEF_{in}$ $HI_{SS.InaIP} = CRS \cdot \frac{EC_{InaI} \cdot PEF_{in}}{RfC}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration IUR$_{Ina}$ = Inhalation Unit Risk RfC$_{Ina}$= Reference concentration EC$_{Inal}$ = Indoor inhalation rate PEF$_{in}$ = Particulate indoor emission factor
Indoor cumulative risk $R_{SS.Indoor} = R_{SS.InaI} + R_{SS.InaIP}$ $HI_{SS.Indoor} = HI_{SS.InaI} + HI_{SS.InaIP}$	
Ingestion of water $R_{SS.LF} = CRS \cdot \frac{SF_{Ing} \cdot EM_{IngW} \cdot LF_{ss}}{DAF}$ $HI_{SS.LF} = CRS \cdot \frac{EM_{IngW} \cdot LF_{ss}}{RfD_{Ing} \cdot DAF}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI$_{ng}$ = Slope factor - ingestion RfD I$_{ng}$ = Reference dose - ingestion EMI$_{ngW}$ = Water Ingestion rate LF$_{ss}$ = Leaching factor DAF = Groundwater dilution factor
Risk and Hazard Index for surface soil $R_{SS} = \max\left[R_{SS.outdoor}; R_{SS.Indoor}; R_{SS.LF}\right]$ $HI_{SS} = \max\left[HI_{SS.outdoor}; HI_{SS.Indoor}; HI_{SS.LF}\right]$	

For On-site Receptors ADF = 1; DAF = 1

Table 10. Subsurface Soil: Risk and Hazard Index

Outdoor Vapor Inhalation
(reference dose method)

$$R_{SP.InaO} = CRS \cdot SF_{Ina} \cdot VF_{samb} \cdot EM_{InaO} \cdot ADF$$

$$HI_{SP.InaO} = CRS \cdot \frac{VF_{samb} \cdot EM_{InaO} \cdot ADF}{RfD_{Ina}}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose - inhalation
EM_{InaO} = Outdoor inhalation rate
VF_{samb} = Outdoor volatilization factor
ADF = Atmospheric dispersion factor

Outdoor Vapor Inhalation
(reference concentration method)

$$R_{SP.InaO} = CRS \cdot IUR_{Ina} \cdot VF_{samb} \cdot EC_{InaO} \cdot ADF$$

$$HI_{SP.InaO} = CRS \cdot \frac{VF_{samb} \cdot EC_{InaO} \cdot ADF}{RfC_{Ina}}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaO} = Outdoor inhalation rate
VF_{samb} = Outdoor volatilization factor
ADF = Atmospheric dispersion factor

Indoor Vapor Inhalation (no off-site)
(reference dose method)

$$R_{SP.InaI} = CRS \cdot SF_{Ina} \cdot VF_{sesp} \cdot EM_{InaI}$$

$$HI_{SP.InaI} = CRS \cdot \frac{VF_{sesp} \cdot EM_{InaI}}{RfD_{Ina}}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose - inhalation
EM_{InaI} = Indoor inhalation rate
VF_{sesp} = Indoor volatilization factor

Indoor Vapor Inhalation (no off-site)
(reference concentration method)

$$R_{SP.InaI} = CRS \cdot IUR_{Ina} \cdot VF_{sesp} \cdot EC_{InaI}$$

$$HI_{SP.InaI} = CRS \cdot \frac{VF_{sesp} \cdot EC_{InaI}}{RfC_{Ina}}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaI} = Indoor inhalation rate
VF_{sesp} = Indoor volatilization factor

Ingestion of water

$$R_{SP.LF} = CRS \cdot \frac{SF_{Ing} \cdot EM_{IngW} \cdot LF_{sp}}{DAF}$$

$$HI_{SP.LF} = CRS \cdot \frac{EM_{IngW} \cdot LF_{sp}}{RfD_{Ing} \cdot DAF}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
SFI_{ng} = Slope factor - ingestion
RfD I_{ng} = Reference dose - ingestion
EMI_{ngW} = Water Ingestion rate
LF_{sp} = Leaching factor
DAF = Groundwater dilution factor

Risk and Hazard Index for subsurface soil

$$R_{SP} = \max\left[R_{SP.InaO}; R_{SP.InaI}; R_{SP.LF}\right]$$

$$HI_{SP} = \max\left[HI_{SP.InaO}; HI_{SP.InaI}; HI_{SP.LF}\right]$$

For On-site Receptors ADF = 1; DAF = 1

Table 11. Groundwater: Risk and Hazard Index

Outdoor Vapor Inhalation ***(reference dose method)*** $R_{GW.InaO} = CRS \cdot \frac{SF_{Ina} \cdot VF_{wamb} \cdot EM_{InaO}}{DAF}$ $HI_{GW.InaO} = CRS \cdot \frac{VF_{wamb} \cdot EM_{InaO}}{RfD_{Ina} \cdot DAF}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI_{na} = Slope factor - inhalation RfD I_{na} = Reference dose - inhalation EM_{InaO} = Outdoor inhalation rate VF_{wamb} = Outdoor volatilization factor DAF = Groundwater dilution factor
Outdoor Vapor Inhalation ***(reference concentration method)*** $R_{GW.InaO} = CRS \cdot \frac{IUR_{Ina} \cdot VF_{wamb} \cdot EC_{InaO}}{DAF}$ $HI_{GW.InaO} = CRS \cdot \frac{VF_{wamb} \cdot EC_{InaO}}{RfC_{Ina} \cdot DAF}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration IUR_{Ina} = Inhalation Unit Risk RfC_{Ina}= Reference concentration EC_{InaO} = Outdoor inhalation rate VF_{wamb} = Outdoor volatilization factor DAF = Groundwater dilution factor
Indoor Vapor Inhalation ***(reference dose method)*** $R_{GW.InaI} = CRS \cdot \frac{SF_{Ina} \cdot VF_{wesp} \cdot EM_{InaI}}{DAF}$ $HI_{GW.InaI} = CRS \cdot \frac{VF_{wesp} \cdot EM_{InaI}}{RfD_{Ina} \cdot DAF}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI_{na} = Slope factor - inhalation RfD I_{na} = Reference dose - inhalation EM_{InaI} = Indoor inhalation rate VF_{wesp} = Indoor volatilization factor DAF = Groundwater dilution factor
Indoor Vapor Inhalation ***(reference concentration method)*** $R_{GW.InaI} = CRS \cdot \frac{IUR_{Ina} \cdot VF_{wesp} \cdot EC_{InaI}}{DAF}$ $HI_{GW.InaI} = CRS \cdot \frac{VF_{wesp} \cdot EC_{InaI}}{RfC_{Ina} \cdot DAF}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration IUR_{Ina} = Inhalation Unit Risk RfC_{Ina}= Reference concentration EC_{InaI} = Indoor inhalation rate VF_{wesp} = Indoor volatilization factor DAF = Groundwater dilution factor
Ingestion of water $R_{GW.D} = CRS \cdot \frac{SF_{Ing} \cdot EM_{IngW}}{DAF}$ $HI_{GW.D} = CRS \cdot \frac{EM_{IngW}}{RfD_{Ing} \cdot DAF}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI_{ng} = Slope factor - ingestion RfD I_{ng} = Reference dose - ingestion EMI_{ngW} = Water Ingestion rate DAF = Groundwater dilution factor
Risk and Hazard Index for groundwater $R_{GW} = \max\left[R_{GW.InaO}; R_{GW.InaI}; R_{GW.D}\right]$ $HI_{GW} = \max\left[HI_{GW.InaO}; HI_{GW.InaI}; HI_{GW.D}\right]$	

For On-site Receptors DAF = 1

Table 12. Risk for the groundwater resource

Surface Soil – Leaching to Groundwater $R_{SS.LF} = \frac{CRS \cdot LF_{ss}}{DAF \cdot MCL_{GW}}$	CRS = Source Concentration MCL_{GW} = Maximum Contaminant Level LF_{ss} = Leaching factor DAF = Groundwater dilution factor
Subsurface Soil – Leaching to Groundwater $R_{SP.LF} = \frac{CRS \cdot LF_{sp}}{DAF \cdot MCL_{GW}}$	CRS = Source Concentration MCL_{GW} = Maximum Contaminant Level LF_{sp} = Leaching factor DAF = Groundwater dilution factor
Affected groundwater $R_{GW.D} = \frac{CRS}{DAF \cdot MCL_{GW}}$	CRS = Source Concentration MCL_{GW} = Maximum Contaminant Level DAF = Groundwater dilution factor

For On-site Receptors DAF = 1

APP. 1B. RISK CALCULATION (BACKFILL MATERIALS)

Table 13. Backfill Materials: Risk and Hazard Index

Soil ingestion (no off-site) $R_{\text{MdR}.IngS} = CRS_{ss} \cdot SF_{Ing} \cdot EM_{IngS} \cdot 10^{-6}\ kg/mg$ $HI_{\text{MdR}.IngS} = CRS_{ss} \cdot \frac{EM_{IngS} \cdot 10^{-6}\ kg/mg}{RfD_{Ing}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI$_{ng}$ = Slope factor - ingestion RfD I$_{ng}$ = Reference dose - ingestion EMI$_{ngs}$ = Soil Ingestion rate
Dermal Contact (no off-site) $R_{\text{MdR}.ConD} = CRS_{ss} \cdot SF_{Ing} \cdot EM_{ConD} \cdot 10^{-6}\ kg/mg$ $HI_{\text{MdR}.ConD} = CRS_{ss} \cdot \frac{EM_{ConD} \cdot 10^{-6}\ kg/mg}{RfD_{Ing}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI$_{ng}$ = Slope factor for ingestion RfD I$_{ng}$ = Reference dose - ingestion EM$_{ConD}$ = Dermal contact rate
Outdoor Vapor Inhalation ***(reference dose method)*** $R_{\text{MdR}.InaO} = CRS_{tot} \cdot SF_{Ina} \cdot EM_{InaO} \cdot VF_{\text{MdR}} \cdot ADF$ $HI_{\text{MdR}.InaO} = CRS_{tot} \cdot \frac{EM_{InaO} \cdot VF_{\text{MdR}} \cdot ADF}{RfD_{Ina}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI$_{na}$ = Slope factor - inhalation RfD I$_{na}$ = Reference dose - inhalation EM$_{InaO}$ = Outdoor inhalation rate VF$_{MdR}$ = Outdoor volatilization factor ADF = Atmospheric dispersion factor
Outdoor Vapor Inhalation ***(reference concentration method)*** $R_{\text{MdR}.InaO} = CRS_{tot} \cdot IUR \cdot EC_{InaO} \cdot VF_{\text{MdR}} \cdot ADF$ $HI_{\text{MdR}.InaO} = CRS_{tot} \cdot \frac{EC_{InaO} \cdot VF_{\text{MdR}} \cdot ADF}{RfC}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration IUR$_{Ina}$ = Inhalation Unit Risk RfC$_{Ina}$= Reference concentration EC$_{InaO}$ = Outdoor inhalation rate VF$_{MdR}$ = Outdoor volatilization factor ADF = Atmospheric dispersion factor
Outdoor Dust Inhalation ***(reference dose method)*** $R_{\text{MdR}.InaOP} = CRS_{ss} \cdot SF_{Ina} \cdot EM_{InaO} \cdot PEF \cdot ADF$ $HI_{\text{MdR}.InaOP} = CRS_{ss} \cdot \frac{EM_{InaO} \cdot PEF \cdot ADF}{RfD_{Ina}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI$_{na}$ = Slope factor - inhalation RfD I$_{na}$ = Reference dose - inhalation EM$_{InaO}$ = Outdoor inhalation rate PEF = Partculate emission factor ADF = Atmospheric dispersion factor
Outdoor Dust Inhalation ***(reference concentration method)*** $R_{\text{MdR}.InaOP} = CRS_{ss} \cdot IUR \cdot EC_{InaO} \cdot PEF \cdot ADF$ $HI_{\text{MdR}.InaOP} = CRS_{ss} \cdot \frac{EC_{InaO} \cdot PEF \cdot ADF}{RfC}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration IUR$_{Ina}$ = Inhalation Unit Risk RfC$_{Ina}$= Reference concentration EC$_{InaO}$ = Outdoor inhalation rate PEF = Partculate emission factor ADF = Atmospheric dispersion factor

Table 13. Backfill Materials: Risk and Hazard Index

Outdoor cumulative risk

$$R_{\mathrm{MdR}.outdoor} = R_{\mathrm{MdR}.IngS} + R_{\mathrm{MdR}.ConD} + R_{\mathrm{MdR}.InaO} + R_{\mathrm{MdR}.InaOP}$$

$$HI_{\mathrm{MdR}.outdoor} = HI_{\mathrm{MdR}.IngS} + HI_{\mathrm{MdR}.ConD} + HI_{\mathrm{MdR}.InaO} + HI_{\mathrm{MdR}.InaOP}$$

Indoor Vapor Inhalation (no off-site)
(reference dose method)

$$R_{\mathrm{MdR}.InaI} = CRS_{tot} \cdot SF_{Ina} \cdot EM_{InaI} \cdot VF_{\mathrm{MdR},esp}$$

$$HI_{\mathrm{MdR}.InaI} = CRS_{tot} \cdot \frac{EM_{InaI} \cdot VF_{\mathrm{MdR},esp}}{RfD_{Ina}}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose - inhalation
EM_{InaI} = Indoor inhalation rate
VF_{MdResp} = Indoor volatilization factor

Indoor Vapor Inhalation (no off-site)
(reference concentration method)

$$R_{\mathrm{MdR}.InaI} = CRS_{tot} \cdot IUR \cdot EC_{InaI} \cdot VF_{\mathrm{MdR},esp}$$

$$HI_{\mathrm{MdR}.InaI} = CRS_{tot} \cdot \frac{EC_{InaI} \cdot VF_{\mathrm{MdR},esp}}{RfC}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaI} = Indoor inhalation rate
VF_{MdResp} = Indoor volatilization factor

Indoor Dust Inhalation (no off-site)
(reference dose method)

$$R_{\mathrm{MdR}.InaIP} = CRS_{ss} \cdot SF_{Ina} \cdot EM_{InaI} \cdot PEF_{in}$$

$$HI_{\mathrm{MdR}.InaIP} = CRS_{ss} \cdot \frac{EM_{InaI} \cdot PEF_{in}}{RfD_{Ina}}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose - inhalation
EM_{InaI} = Indoor inhalation rate
PEF_{in} = Particulate indoor emission factor

Indoor Dust Inhalation (no off-site)
(reference concentration method)

$$R_{\mathrm{MdR}.InaIP} = CRS_{ss} \cdot IUR \cdot EC_{InaI} \cdot PEF_{in}$$

$$HI_{\mathrm{MdR}.InaIP} = CRS_{ss} \cdot \frac{EC_{InaI} \cdot PEF_{in}}{RfC}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaI} = Indoor inhalation rate
PEF_{in} = Particulate indoor emission factor

Indoor cumulative risk

$$R_{\mathrm{MdR}.Indoor} = R_{\mathrm{MdR}.InaI} + R_{\mathrm{MdR}.InaIP}$$

$$HI_{\mathrm{MdR}.Indoor} = HI_{\mathrm{MdR}.InaI} + HI_{\mathrm{MdR}.InaIP}$$

Ingestion of water

$$R_{\mathrm{MdR}.LF} = CRS_{tot} \cdot \frac{SF_{Ing} \cdot EM_{IngW} \cdot LF_{\mathrm{MdR}}}{DAF}$$

$$HI_{\mathrm{MdR}.LF} = CRS_{tot} \cdot \frac{EM_{IngW} \cdot LF_{\mathrm{MdR}}}{RfD_{Ing} \cdot DAF}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
SFI_{ng} = Slope factor - ingestion
RfD I_{ng} = Reference dose - ingestion
EMI_{ngW} = Water Ingestion rate
LF_{MdR} = Leaching factor
DAF = Groundwater dilution

Risk and Hazard Index for Backfill Materials

$$R_{\mathrm{MdR}} = \max\left[R_{\mathrm{MdR}.outdoor}; R_{\mathrm{MdR}.Indoor}; R_{\mathrm{MdR}.LF}\right]$$

$$HI_{\mathrm{MdR}} = \max\left[HI_{\mathrm{MdR}.outdoor}; HI_{\mathrm{MdR}.Indoor}; HI_{\mathrm{MdR}.LF}\right]$$

For On-site Receptors ADF = 1; DAF = 1

Table 14. Backfill Material: risk for the groundwater resource

Leaching from Backfill Material

$$R_{\mathrm{MdR}.LF} = \frac{CRS_{tot} \cdot LF_{MdR}}{DAF \cdot MCL_{GW} \cdot 10^{-3}\ mg/\mu g}$$

CRS = Source Concentration
MCL_{GW} = Maximum Contaminant Level
L_{sMdR} = Leaching factor
DAF = Groundwater dilution factor

For On-site Receptors DAF = 1

Table 15. Eluate Backfill Material: Risk and Hazard Index

Water Ingestion

$$R_{EL,MdR.D} = CRS \cdot \frac{\alpha_{LF,MdR} \cdot SF_{Ing} \cdot EM_{IngW}}{DAF}$$

$$HI_{EL,Md.D} = CRS \cdot \frac{\alpha_{LF,MdR} \cdot EM_{IngW}}{RfD_{Ing} \cdot DAF}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Source Concentration
SFI_{ng} = Slope factor - ingestion
RfD I_{ng} = Reference dose - ingestion
EMI_{ngW} = Water Ingestion rate
$\alpha_{LF,MdR}$ = Leaching factor
DAF = Groundwater dilution factor

Leaching from Backfill Material

$$R_{GW.EL,MdR} = \frac{CRS \cdot \alpha_{LF,MdR}}{DAF \cdot MCL_{GW} \cdot 10^{-3}\ mg/\mu g}$$

CRS = Source Concentration
MCL_{GW} = Maximum Contaminant Level
$\alpha_{LF,MdR}$ = Leaching factor
DAF = Groundwater dilution factor

APP. 1C. RISK CALCULATION (INT. CHARACTERIZATION)

Table 16. Soil-gas: Risk and Hazard Index

Outdoor Vapor Inhalation ***(reference dose method)*** $R_{SG.InaO} = CRS \cdot SF_{Ina} \cdot \alpha_{samb} \cdot EM_{InaO} \cdot ADF$ $HI_{SG.InaO} = CRS \cdot \frac{\alpha_{samb} \cdot EM_{InaO} \cdot ADF}{RfD_{Ina}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Representative Concentration SFI_{na} = Slope factor - inhalation RfD I_{na} = Reference dose - inhalation EM_{InaO} = Outdoor inhalation rate α_{samb} = Outdoor volatilization factor ADF = Atmospheric dispersion factor
Outdoor Vapor Inhalation ***(reference concentration method)*** $R_{SG.InaO} = CRS \cdot IUR \cdot \alpha_{samb} \cdot EC_{InaO} \cdot ADF$ $HI_{SG.InaO} = CRS \cdot \frac{\alpha_{samb} \cdot EC_{InaO} \cdot ADF}{RfC}$	R = Carcinogenic Risk HI = Hazard Index CRS = Representative Concentration IUR_{Ina} = Inhalation Unit Risk RfC_{Ina}= Reference concentration EC_{InaO} = Outdoor inhalation rate α_{samb} = Outdoor volatilization factor ADF = Atmospheric dispersion factor
Indoor Vapor Inhalation ***(reference dose method)*** $R_{SG.InaI} = CRS \cdot SF_{Ina} \cdot \alpha_{sesp} \cdot EM_{InaI}$ $HI_{SG.InaI} = CRS \cdot \frac{\alpha_{sesp} \cdot EM_{InaI}}{RfD_{Ina}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Representative Concentration SFI_{na} = Slope factor - inhalation RfD I_{na} = Reference dose - inhalation EM_{InaI} = Indoor inhalation rate α_{samb} = Indoor volatilization factor
Indoor Vapor Inhalation ***(reference concentration method)*** $R_{SG.InaI} = CRS \cdot IUR \cdot \alpha_{sesp} \cdot EC_{InaI}$ $HI_{SG.InaI} = CRS \cdot \frac{\alpha_{sesp} \cdot EC_{InaI}}{RfC}$	R = Carcinogenic Risk HI = Hazard Index CRS = Representative Concentration IUR_{Ina} = Inhalation Unit Risk RfC_{Ina}= Reference concentration EC_{InaI} = Indoor inhalation rate α_{samb} = Indoor volatilization factor

For On-site Receptors ADF = 1

Table 17. Flux-Chambers: Risk and Hazard Index

Outdoor Vapor Inhalation - Concentration
(reference dose method)

$$R_{FC.InaO} = CRS \cdot SF_{Ina} \cdot \alpha_{FC} \cdot EM_{InaO} \cdot ADF$$

$$HI_{FC.InaO} = CRS \cdot \frac{\alpha_{FC} \cdot EM_{InaO} \cdot ADF}{RfD_{Ina}}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Representative Concentration
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose - inhalation
EM_{InaO} = Outdoor inhalation rate
α_{FC} = Outdoor volatilization factor
ADF = Atmospheric dispersion factor

Outdoor Vapor Inhalation - Flux
(reference concentration method)

$$R_{FC.InaO} = CRS \cdot IUR \cdot \alpha_{FC} \cdot EC_{InaO} \cdot ADF$$

$$HI_{FC.InaO} = CRS \cdot \frac{\alpha_{FC} \cdot EC_{InaO} \cdot ADF}{RfC}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Representative Concentration
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaO} = Outdoor inhalation rate
α_{FC} = Outdoor volatilization factor
ADF = Atmospheric dispersion factor

Outdoor Vapor Inhalation - Concentration
(reference dose method)

$$R_{FC.InaO} = F \cdot SF_{Ina} \cdot \alpha_{FC(flux)} \cdot EM_{InaO} \cdot ADF$$

$$HI_{FC.InaO} = F \cdot \frac{\alpha_{FC(flux)} \cdot EM_{InaO} \cdot ADF}{RfD_{Ina}}$$

R = Carcinogenic Risk
HI = Hazard Index
F = Measured Flux
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose - inhalation
EM_{InaO} = Outdoor inhalation rate
$\alpha_{FC(flux)}$ = Outdoor volatilization factor
ADF = Atmospheric dispersion factor

Outdoor Vapor Inhalation - Flux
(reference concentration method)

$$R_{FC.InaO} = F \cdot IUR \cdot \alpha_{FC(flux)} \cdot EC_{InaO} \cdot ADF$$

$$HI_{FC.InaO} = F \cdot \frac{\alpha_{FC(flux)} \cdot EC_{InaO} \cdot ADF}{RfC}$$

R = Carcinogenic Risk
HI = Hazard Index
F = Measured Flux
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaO} = Outdoor inhalation rate
$\alpha_{FC(flux)}$ = Outdoor volatilization factor
ADF = Atmospheric dispersion factor

For On-site Receptors ADF = 1

Table 18. Ambient Air measurements: Risk and Hazard Index	
Outdoor Vapor Inhalation ***(reference dose method)*** $R_{AR.InaO} = CRS \cdot SF_{Ina} \cdot EM_{InaO} \cdot ADF$ $HI_{AR.InaO} = CRS \cdot \frac{EM_{InaO} \cdot ADF}{RfD_{Ina}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Representative Concentration SFI_{na} = Slope factor - inhalation RfD I_{na} = Reference dose - inhalation EM_{InaO} = Outdoor inhalation rate ADF = Atmospheric dispersion factor
Outdoor Vapor Inhalation ***(reference concentration method)*** $R_{AR.InaO} = CRS \cdot IUR \cdot EC_{InaO} \cdot ADF$ $HI_{AR.InaO} = CRS \cdot \frac{EC_{InaO} \cdot ADF}{RfC}$	R = Carcinogenic Risk HI = Hazard Index CRS = Representative Concentration IUR_{Ina} = Inhalation Unit Risk RfC_{Ina}= Reference concentration EC_{InaO} = Outdoor inhalation rate ADF = Atmospheric dispersion factor
Indoor Vapor Inhalation ***(reference dose method)*** $R_{AR.InaI} = CRS \cdot SF_{Ina} \cdot EM_{InaI}$ $HI_{AR.InaI} = CRS \cdot \frac{EM_{InaI}}{RfD_{Ina}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Representative Concentration SFI_{na} = Slope factor - inhalation RfD I_{na} = Reference dose - inhalation EM_{InaI} = Indoor inhalation rate
Indoor Vapor Inhalation ***(reference concentration method)*** $R_{AR.InaI} = CRS \cdot IUR \cdot EC_{InaI}$ $HI_{AR.InaI} = CRS \cdot \frac{EC_{InaI}}{RfC}$	R = Carcinogenic Risk HI = Hazard Index CRS = Representative Concentration IUR_{Ina} = Inhalation Unit Risk RfC_{Ina}= Reference concentration EC_{InaI} = Indoor inhalation rate

For On-site Receptors ADF = 1

Table 19. Eluate (Surface Soil): Risk and Hazard Index

Water Ingestion

$$R_{ELss.D} = CRS \cdot \frac{\alpha_{LFss} \cdot SF_{Ing} \cdot EM_{IngW}}{DAF}$$

$$HI_{ELss.D} = CRS \cdot \frac{\alpha_{LFss} \cdot EM_{IngW}}{RfD_{Ing} \cdot DAF}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Representative Concentration
SF_{Ing} = Slope factor - ingestion
RfD_{Ing} = Reference dose - ingestion
EM_{IngW} = Water Ingestion rate
α_{LFss} = Leaching Factor
DAF = Dilution Attenuation Factor

Groundwater Protection

$$R_{GW.ELss} = \frac{CRS \cdot \alpha_{LFss}}{DAF \cdot MCL_{GW}}$$

CRS = Representative Concentration
MCL_{GW} = Maximum contaminant level
α_{LFss} = Leaching Factor
DAF = Dilution Attenuation Factor

For On-site Receptors *DAF=1*

Table 20. Eluate (Subsurface Soil): Risk and Hazard Index

Water Ingestion

$$R_{ELsp.D} = CRS \cdot \frac{\alpha_{LFsp} \cdot SF_{Ing} \cdot EM_{IngW}}{DAF}$$

$$HI_{ELsp.D} = CRS \cdot \frac{\alpha_{LFsp} \cdot EM_{IngW}}{RfD_{Ing} \cdot DAF}$$

R = Carcinogenic Risk
HI = Hazard Index
CRS = Representative Concentration
SF_{Ing} = Slope factor - ingestion
RfD_{Ing} = Reference dose - ingestion
EM_{IngW} = Water Ingestion rate
α_{LFsp} = Leaching Factor
DAF = Dilution Attenuation Factor

Groundwater Protection

$$R_{GW.ELsp} = \frac{CRS \cdot \alpha_{LFsp}}{DAF \cdot MCL_{GW}}$$

CRS = Representative Concentration
MCL_{GW} = Maximum contaminant level
α_{LFsp} = Leaching Factor
DAF = Dilution Attenuation Factor

For On-site Receptors *DAF=1*

APP. 1D. RISK CALCULATION (AGRI-FOOD CONSUMPTION)

Table 21. Risk calculation for agri-food consumption

Average e Lifetime Average Daily Dose (ADD e LADD) $ADD = [\sum_i (C \times IR)_i \times EF \times ED]/(BW \times AT_{ADD} \times 365)$ $LADD = [\sum_i (C \times IR)_i \times EF \times ED]/(BW \times AT_{LADD} \times 365)$ *This calculation is performed for each receptor (child, teenager, adult and senior)*	C = Concentration in the agri-food product IR = Food consumption rate EF = exposure frequency ED = exposure duration BW = body weight AT_{ADD} = average time for non-carcinogenic contaminants AT_{LADD} = average time for carcinogenic contaminants
Risk and Hazard Index $HI = ADD/RfD$ $R = LADD \times SF$ *This calculation is performed for each receptor (child, teenager, adult and senior)*	R = Carcinogenic Risk HI = Hazard Index ADD = Average Daily Dose LADD = Lifetime Average Daily Dose RfD = Reference Dose Ingestion SF = Slope Factor Ingestion

APP. 2A. CLEAN-UP LEVELS CALCULATION (SSTL)

The calculation of the remediation targets (Individual Site-Specific Target Levels, SSTL) is performed by the application of the risk analysis procedure in backward mode. The clean-up levels calculated represent the maximum acceptable concentration in the affected source medium (soil or groundwater) that is protective of a human or groundwater receptor located at a relevant point of exposure.

Individual Clean-up Levels (SSTL). The calculation of the clean-up levels (*SSTL*) is performed using the same equations applied to calculate the risk, properly reversed and expressed in terms of the source concentration:

$$SSTL = \frac{C_{poe}}{FT} = \frac{E}{EM \cdot FT} = \frac{TR}{SF \cdot EM \cdot FT}$$

carcinogenic contaminants

$$SSTL = \frac{Cpoe}{FT} = \frac{E}{EM \cdot FT} = \frac{THI \cdot RfD}{EM \cdot FT}$$

non-carcinogenic contaminants

Where:
TR: Target Risk for the single constituent (e.g. TR = 10^{-6})
THI: Target Hazard Index for the single constituent (THI = 1)
E: daily chronic contaminant exposure rate
SF: Slope Factor
RfD: Reference Dose
C_{poe}: Concentration at the point of exposure
EM: Intake rate
FT: Fate & Transport factor

This calculation is repeated for the different exposure and migration pathways active in the site using the appropriate exposure factors and transport (for details, see the tables below). The equations for the different F&T factors and intake rates are reported in the next paragraphs.

Note that the above equations are those reported in the ISPRA guidelines (2008) that are based on the use of the Reference Dose (RfD) and the Slope Factor (SF). However, for the inhalation pathway the software allows the user to use the approach based on the Reference Concentration (RfC) and the Inhalation Unit Risk (IUR) using the following equations:

$$SSTL = \frac{TR}{IUR \cdot EC \cdot FT}$$ carcinogenic contaminants

$$SSTL = \frac{THI \cdot RfC}{EC \cdot FT}$$ non-carcinogenic contaminants

In the following tables, the equations implemented in the software are distinguished as “reference dose method” and “reference concentration method”

Multiple exposure pathways. The equations described above provide an assessment of the *SSTL* for the single exposure pathway. The Individual *SSTL* (associated to the single contaminant) is derived by cumulating the effects of the different exposure scenarios (e.g. Outdoor exposure) and then choosing the most conservative value (i.e. the lower value) between the *SSTL* calculated for the different scenarios. Namely, the combined effect of multiple exposure is estimated as the reciprocal of the sum of the reciprocals of the *SSTL* calculated for each route of exposure. Let assume, for example, the case of *SSTL* for the calculation of exposure in outdoor environments:

$$SSTL_{outdoor} = \frac{1}{1/SSTL_{ing} + 1/SSTL_{derm.cont} + 1/SSTL_{dusts} + 1/SSTL_{vapors}} \tag{12}$$

For other scenarios, see the tables below.

The following figures report the criteria used in the software for the calculation of the individual clean-up levels for each media of concern accounting for multiple exposure pathways.

SURFACE SOIL

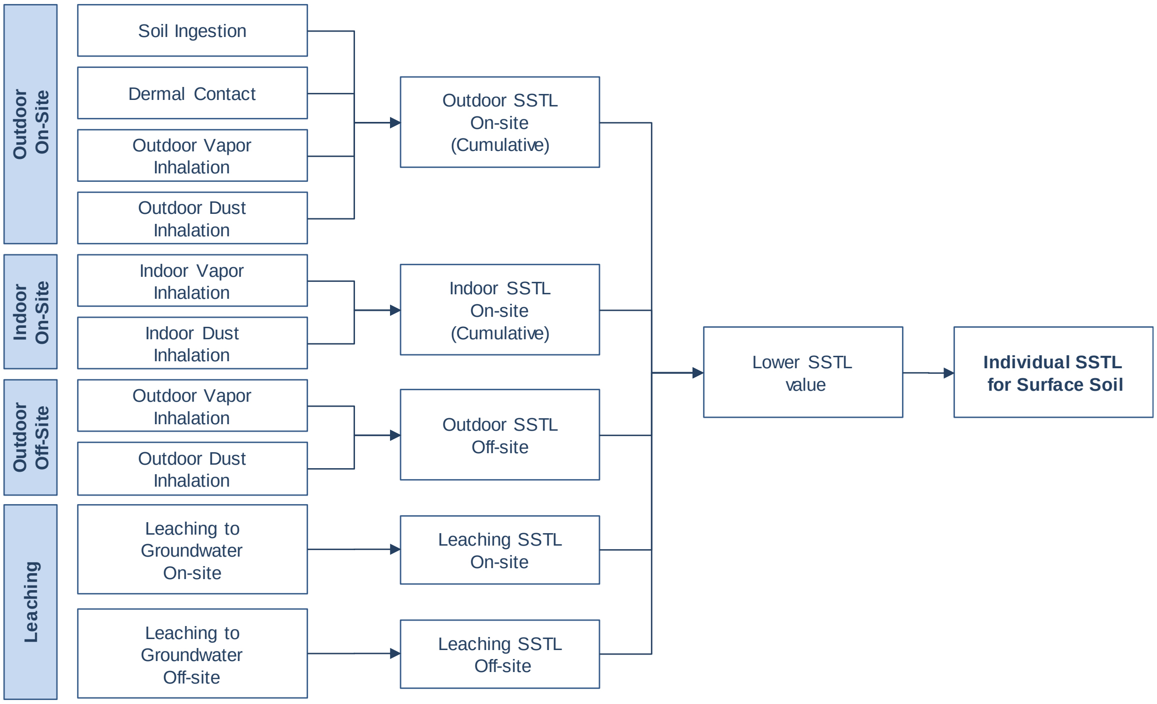

Figure 36. *SSTL* – Surface soil. Multiple exposures.

SUBSURFACE SOIL

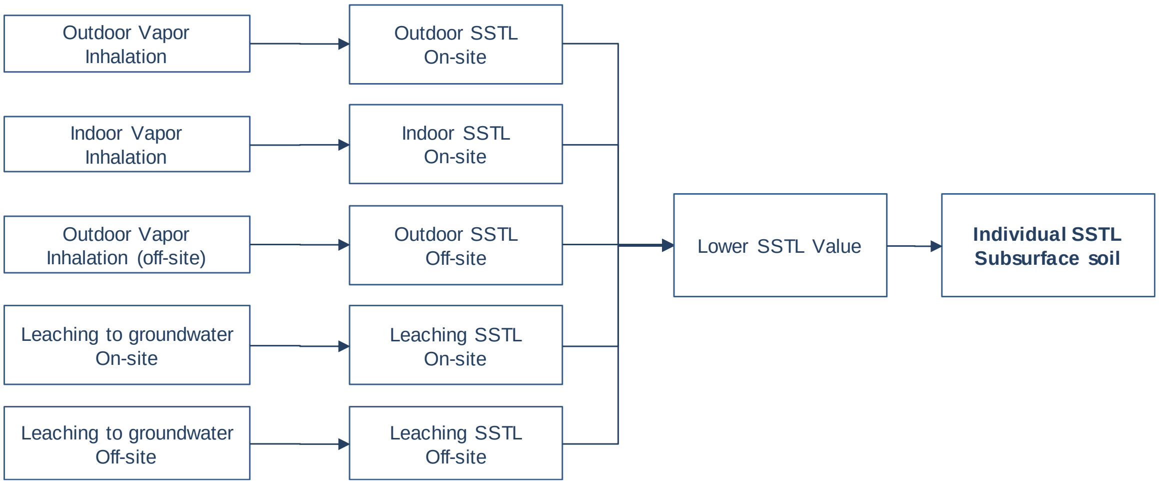

Figure 37. *SSTL* – Subsurface soil. Multiple exposures.

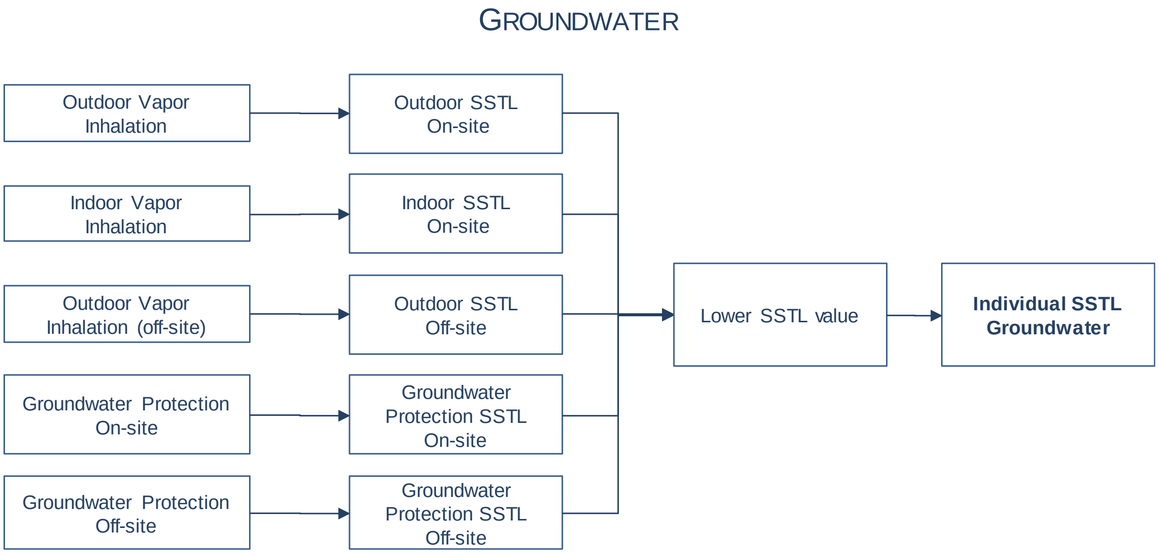

Figure 38. *SSTL* – Groundwater. Multiple exposures.

Cumulative SSTL (Clean-up levels). The *SSTL* calculated above does not constitute yet the remediation targets since these concentrations only meet the condition of tolerable risk for exposure to a single contaminant. In fact, the individual *SSTL* does not necessarily meet the requirement of cumulative target risk. Thus, to account for the effects of the cumulative risk, it is necessary to further reduce the individual *SSTL* to ensure the achievement of values of concentration such that the condition of acceptable cumulative risk is met:

$$\sum_{i}^{n} SSTL_i^{cum} \cdot FT_i \cdot EM_i \cdot SF_i \leq TR \qquad \text{for carcinogenic contaminants}$$

$$\sum_{i}^{n} \frac{SSTL_i^{cum} \cdot FT_i \cdot EM_i}{RfD_i} \leq THI \qquad \text{for non carcinogenic contaminants}$$

The *SSTL* that meet both the individual and cumulative target limits represent the site-specific clean-up levels for the contaminated matrix.

Table 22. Surface Soil: SSTL

Soil Ingestion (no off-site)

$$SSTL_{SS.Ing} = \min \begin{cases} SSTL_{canc} = \dfrac{TR}{SF_{Ing} \cdot EM_{IngS} \cdot 10^{-6}\ kg/mg} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfD_{Ing}}{EM_{IngS} \cdot 10^{-6}\ kg/mg} \end{cases}$$

SSTL_{canc} = SSTL carcinogenic cont.
$\mathrm{SSTL}_{non \cdot canc}$ = SSTL non-carcinogenic
TR = Target Risk
THQ = Target Hazard Index
SFI_{ng} = Slope factor - ingestion
RfD I_{ng} = Reference dose - ingestion
EMI_{ngs} = Soil Ingestion rate

Dermal Contact (no off-site)

$$SSTL_{SS.ConD} = \min \begin{cases} SSTL_{canc} = \dfrac{TR}{SF_{Ing} \cdot EM_{ConD} \cdot 10^{-6}\ kg/mg} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfD_{Ing}}{EM_{ConD} \cdot 10^{-6}\ kg/mg} \end{cases}$$

SSTL_{canc} = SSTL carcinogenic cont.
$\mathrm{SSTL}_{non \cdot canc}$ = SSTL non-carcinogenic
TR = Target Risk
THQ = Target Hazard Index
SFI_{ng} = Slope factor - ingestion
RfD I_{ng} = Reference dose - ingestion
EM_{ConD} = Dermal contact rate

Outdoor Vapors Inhalation
(reference dose method)

$$SSTL_{SS.InaO} = \min \begin{cases} SSTL_{canc} = \dfrac{TR}{SF_{Ina} \cdot EM_{InaO} \cdot VF_{ss} \cdot ADF} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfD_{Ina}}{EM_{InaO} \cdot VF_{ss} \cdot ADF} \end{cases}$$

SSTL_{canc} = SSTL carcinogenic cont.
$\mathrm{SSTL}_{non \cdot canc}$ = SSTL non-carcinogenic
TR = Target Risk
THQ = Target Hazard Index
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose – inhalation
EM_{InaO} = Outdoor inhalation rate
VF_{ss} = Outdoor Volatilization factor
ADF = Atmospheric dispersion factor

Outdoor Vapors Inhalation
(reference concentration method)

$$SSTL_{SS.InaO} = \min \begin{cases} SSTL_{canc} = \dfrac{TR}{IUR_{Ina} \cdot EC_{InaO} \cdot VF_{ss} \cdot ADF} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfC_{Ina}}{EC_{InaO} \cdot VF_{ss} \cdot ADF} \end{cases}$$

SSTL_{canc} = SSTL carcinogenic cont.
$\mathrm{SSTL}_{non \cdot canc}$ = SSTL non-carcinogenic
TR = Target Risk
THQ = Target Hazard Index
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaO} = Outdoor inhalation rate
VF_{ss} = Outdoor Volatilization factor
ADF = Atmospheric dispersion factor

Outdoor Dusts Inhalation
(reference dose method)

$$SSTL_{SS.InaOP} = \min \begin{cases} SSTL_{canc} = \dfrac{TR}{SF_{Ina} \cdot EM_{InaO} \cdot PEF \cdot ADF} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfD_{Ina}}{EM_{InaO} \cdot PEF \cdot ADF} \end{cases}$$

SSTL_{canc} = SSTL carcinogenic cont.
$\mathrm{SSTL}_{non \cdot canc}$ = SSTL non-carcinogenic
TR = Target Risk
THQ = Target Hazard Index
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose - inhalation
EM_{InaO} = Outdoor inhalation rate
PEF = Particulate emission factor
ADF = Atmospheric dispersion factor

Table 22. Surface Soil: SSTL

Outdoor Dusts Inhalation
(reference concentration method)

$$SSTL_{SS.InaOP}=\min\begin{cases} SSTL_{canc}=\dfrac{TR}{IUR_{Ina}\cdot EC_{InaO}\cdot PEF\cdot ADF}\\ SSTL_{non.canc}=\dfrac{THQ\cdot RfC_{Ina}}{EC_{InaO}\cdot PEF\cdot ADF}\end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\text{-}canc}$ = SSTL non-carcinogenic
TR = Target Risk
THQ = Target Hazard Index
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose - inhalation
EM_{InaO} = Outdoor inhalation rate
PEF = Particulate emission factor
ADF = Atmospheric dispersion factor

Outdoor

$$SSTL_{SS.outdoor}=\begin{cases}\dfrac{1}{\dfrac{1}{SSTL_{SS.IngS}}+\dfrac{1}{SSTL_{SS.ConD}}+\dfrac{1}{SSTL_{SS.InaO}}+\dfrac{1}{SSTL_{SS.InaOP}}} & (\text{for } SSTL_{InaO}\le C_{sat})\\ \dfrac{TR-R_{\max,InaO}}{\dfrac{TR}{SSTL_{SS.IngS}}+\dfrac{TR}{SSTL_{SS.ConD}}+\dfrac{TR}{SSTL_{SS.InaOP}}} & (\text{for } SSTL_{InaO}> C_{sat})\end{cases}$$

$$R_{\max,InaO}=\left(C_{sat}/SSTL_{InaO}\right)\cdot TR \qquad (\text{for } SSTL_{InaO}> C_{sat})$$

Indoor Vapors Inhalation (no off-site)
(reference dose method)

$$SSTL_{SS.InaI}=\min\begin{cases} SSTL_{canc}=\dfrac{TR}{SF_{Ina}\cdot EM_{InaI}\cdot VF_{ssesp}}\\ SSTL_{non.canc}=\dfrac{THQ\cdot RfD_{Ina}}{EM_{InaI}\cdot VF_{ssesp}}\end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\text{-}canc}$ = SSTL non-carcinogenic
TR = Target Risk
THQ = Target Hazard Index
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose - inhalation
EM_{InaI} = Indoor inhalation rate
VF_{sesp} = Indoor Volatilization factor

Indoor Vapors Inhalation (no off-site)
(reference concentration method)

$$SSTL_{SS.InaI}=\min\begin{cases} SSTL_{canc}=\dfrac{TR}{IUR_{Ina}\cdot EC_{InaI}\cdot VF_{ssesp}}\\ SSTL_{non.canc}=\dfrac{THQ\cdot RfC_{Ina}}{EC_{InaI}\cdot VF_{ssesp}}\end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\text{-}canc}$ = SSTL non-carcinogenic
TR = Target Risk
THQ = Target Hazard Index
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaI} = Indoor inhalation rate
VF_{sesp} = Indoor Volatilization factor

Indoor Dusts Inhalation (no off-site)
(reference dose method)

$$SSTL_{SS.InaIP}=\min\begin{cases} SSTL_{canc}=\dfrac{TR}{SF_{Ina}\cdot EM_{InaI}\cdot PEF_{in}}\\ SSTL_{non.canc}=\dfrac{THQ\cdot RfD_{Ina}}{EM_{InaI}\cdot PEF_{in}}\end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\text{-}canc}$ = SSTL non-carcinogenic
TR = Target Risk
THQ = Target Hazard Index
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose - inhalation
EM_{InaI} = Indoor inhalation rate
PEF_{in} = Particulate indoor emission factor

Table 22. Surface Soil: SSTL

Indoor Dusts Inhalation (no off-site)
(reference concentration method)

$$SSTL_{SS.InaIP} = \min \begin{cases} SSTL_{canc} = \dfrac{TR}{IUR_{Ina} \cdot EC_{InaI} \cdot PEF_{in}} \\[2ex] SSTL_{non.canc} = \dfrac{THQ \cdot RfC_{Ina}}{EC_{InaI} \cdot PEF_{in}} \end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\cdot canc}$ = SSTL non-carcinogenic
TR = Target Risk
THQ = Target Hazard Index
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina} = Reference concentration
EC_{Inal} = Indoor inhalation rate
PEF_{in} = Particulate indoor emission factor

Indoor

$$SSTL_{SS.Indoor} = \begin{cases} \dfrac{1}{\dfrac{1}{SSTL_{SS.InaI}} + \dfrac{1}{SSTL_{SS.InaIP}}} & (\text{for } SSTL_{InaI} \le C_{sat}) \\[3ex] \dfrac{TR - R_{\max,InaI}}{\dfrac{TR}{SSTL_{SS.InaIP}}} & (\text{for } SSTL_{InaI} > C_{sat}) \end{cases}$$

$$R_{\max,InaI} = \left(C_{sat} / SSTL_{InaI}\right) \cdot TR \qquad (\text{for } SSTL_{InaI} > C_{sat})$$

Leaching to groundwater

$$SSTL_{SS.LF} = \min \begin{cases} SSTL_{canc} = \dfrac{TR \cdot DAF}{SF_{Ing} \cdot EM_{IngW} \cdot LF_{ss}} \\[2ex] SSTL_{non.canc} = \dfrac{THQ \cdot RfD_{Ing} \cdot DAF}{EM_{IngW} \cdot LF_{ss}} \end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\cdot canc}$ = SSTL non-carcinogenic
TR = Target Risk
THQ = Target Hazard Index
SFI_{ng} = Slope factor - ingestion
RfD I_{ng} = Reference dose - ingestion
EMI_{ngW} = Water ingestion rate
LF_{ss} = Leaching Factor
DAF = Groundwater dilution factor

SSTL – Surface Soil

$$SSTL_{SS} = \min\left[SSTL_{SS.outdoor}; SSTL_{SS.Indoor}; SSTL_{SS.LF}\right]$$

For On-site Receptors ADF = 1; DAF = 1

Table 23. Subsurface Soil: SSTL

Outdoor Vapors Inhalation
(reference dose method)

$$SSTL_{SP.InaO} = \min \begin{cases} SSTL_{canc} = \dfrac{TR}{SF_{Ina} \cdot VF_{samb} \cdot EM_{InaO} \cdot ADF} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfD_{Ina}}{VF_{samb} \cdot EM_{InaO} \cdot ADF} \end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\text{-}canc}$ = SSTL non-carcinogenic cont.
TR = Target Risk
THQ = Target Hazard Index
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose – inhalation
EM_{InaO} = Outdoor inhalation rate
VF_{samb} = Outdoor Volatilization factor
ADF = Atmospheric dispersion factor

Outdoor Vapors Inhalation
(reference concentration method)

$$SSTL_{SP.InaO} = \min \begin{cases} SSTL_{canc} = \dfrac{TR}{IUR_{Ina} \cdot VF_{samb} \cdot EC_{InaO} \cdot ADF} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfC_{Ina}}{VF_{samb} \cdot EC_{InaO} \cdot ADF} \end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\text{-}canc}$ = SSTL non-carcinogenic cont.
TR = Target Risk
THQ = Target Hazard Index
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaO} = Outdoor inhalation rate
VF_{samb} = Outdoor Volatilization factor
ADF = Atmospheric dispersion factor

Indoor Vapors Inhalation (no off-site)
(reference dose method)

$$SSTL_{SP.InaI} = \min \begin{cases} SSTL_{canc} = \dfrac{TR}{SF_{Ina} \cdot VF_{sesp} \cdot EM_{InaI}} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfD_{Ina}}{VF_{sesp} \cdot EM_{InaI}} \end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\text{-}canc}$ = SSTL non-carcinogenic cont.
TR = Target Risk
THQ = Target Hazard Index
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose – inhalation
EM_{InaI} = Indoor inhalation rate
VF_{sesp} = Indoor Volatilization factor

Indoor Vapors Inhalation (no off-site)
(reference concentration method)

$$SSTL_{SP.InaI} = \min \begin{cases} SSTL_{canc} = \dfrac{TR}{IUR_{Ina} \cdot VF_{sesp} \cdot EC_{InaI}} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfC_{Ina}}{VF_{sesp} \cdot EC_{InaI}} \end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\text{-}canc}$ = SSTL non-carcinogenic cont.
TR = Target Risk
THQ = Target Hazard Index
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaI} = Indoor inhalation rate
VF_{sesp} = Indoor Volatilization factor

Leaching to groundwater

$$SSTL_{SP.LF} = \min \begin{cases} SSTL_{canc} = \dfrac{TR \cdot DAF}{SF_{Ing} \cdot EM_{IngW} \cdot LF_{sp}} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfD_{Ing} \cdot DAF}{EM_{IngW} \cdot LF_{sp}} \end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\text{-}canc}$ = SSTL non-carcinogenic cont.
TR = Target Risk
THQ = Target Hazard Index
SFI_{ng} = Slope factor - ingestion
RfD I_{ng} = Reference dose - ingestion
EMI_{ngW} = Water ingestion rate
LF_{sp} = Leaching factor
DAF = Groundwater dilution factor

SSTL – Subsurface Soil

$$SSTL_{SP} = \min \left[SSTL_{SP.InaO} ; SSTL_{SP.InaI} ; SSTL_{SP.LF} \right]$$

For On-site Receptors ADF = 1; DAF = 1

Table 24. Groundwater: SSTL

Outdoor Vapors Inhalation
(reference dose method)

$$SSTL_{GW.InaO} = \min\begin{cases} SSTL_{canc} = \dfrac{TR \cdot DAF}{SF_{Ina} \cdot VF_{wamb} \cdot EM_{InaO}} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfD_{Ina} \cdot DAF}{VF_{wamb} \cdot EM_{InaO}} \end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\cdot canc}$ = SSTL non-carcinogenic cont.
TR = Target Risk
THQ = Target Hazard Index
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose – inhalation
EM_{InaO} = Outdoor inhalation rate
VF_{wamb} = Outdoor Volatilization factor
DAF = Groundwater dilution factor

Outdoor Vapors Inhalation
(reference concentration method)

$$SSTL_{GW.InaO} = \min\begin{cases} SSTL_{canc} = \dfrac{TR \cdot DAF}{IUR_{Ina} \cdot VF_{wamb} \cdot EC_{InaO}} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfC_{Ina} \cdot DAF}{VF_{wamb} \cdot EC_{InaO}} \end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\cdot canc}$ = SSTL non-carcinogenic cont.
TR = Target Risk
THQ = Target Hazard Index
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaO} = Outdoor inhalation rate
VF_{wamb} = Outdoor Volatilization factor
DAF = Groundwater dilution factor

Indoor Vapors Inhalation
(reference dose method)

$$SSTL_{GW.InaI} = \min\begin{cases} SSTL_{canc} = \dfrac{TR \cdot DAF}{SF_{Ina} \cdot VF_{wesp} \cdot EM_{InaI}} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfD_{Ina} \cdot DAF}{VF_{wesp} \cdot EM_{InaI}} \end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\cdot canc}$ = SSTL non-carcinogenic cont.
TR = Target Risk
THQ = Target Hazard Index
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose – inhalation
EM_{InaI} = Indoor inhalation rate
VF_{wesp} = Indoor Volatilization factor
DAF = Groundwater dilution factor

Indoor Vapors Inhalation
(reference concentration method)

$$SSTL_{GW.InaI} = \min\begin{cases} SSTL_{canc} = \dfrac{TR \cdot DAF}{IUR_{Ina} \cdot VF_{wesp} \cdot EC_{InaI}} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfC_{Ina} \cdot DAF}{VF_{wesp} \cdot EC_{InaI}} \end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\cdot canc}$ = SSTL non-carcinogenic cont.
TR = Target Risk
THQ = Target Hazard Index
IUR_{Ina} = Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaI} = Indoor inhalation rate
VF_{wesp} = Indoor Volatilization factor
DAF = Groundwater dilution factor

Water Ingestion

$$SSTL_{GW.D} = \min\begin{cases} SSTL_{canc} = \dfrac{TR \cdot DAF}{SF_{Ing} \cdot EM_{IngW}} \\ SSTL_{non.canc} = \dfrac{THQ \cdot RfD_{Ing} \cdot DAF}{EM_{IngW}} \end{cases}$$

$SSTL_{canc}$ = SSTL carcinogenic cont.
$SSTL_{non\cdot canc}$ = SSTL non-carcinogenic cont.
TR = Target Risk
THQ = Target Hazard Index
SFI_{ng} = Slope factor - ingestion
RfD I_{ng} = Reference dose - ingestion
EMI_{ngW} = Water ingestion rate
DAF = Groundwater dilution factor

SSTL - Groundwater

$$SSTL_{GW} = \min\left[SSTL_{GW.InaO}; SSTL_{GW.InaI}; SSTL_{GW.D}\right]$$

For On-site Receptors DAF = 1

Table 25. SSTL Groundwater Resource	
Surface Soil – Leaching to Groundwater $SSTL_{SS.LF} = \frac{MCL_{GW} \cdot DAF}{LF_{ss}}$	MCL_{GW} = Maximum contaminant level LF_{ss} = Leaching factor DAF = Groundwater dilution factor
Subsurface Soil – Leaching to Groundwater $SSTL_{SP.LF} = \frac{MCL_{gw} \cdot DAF}{LF_{sp}}$	MCL_{GW} = Maximum contaminant level LF_{sp} = Leaching factor DAF = Groundwater dilution factor
Affected Groundwater $SSTL_{GW.D} = DAF \cdot MCL_{GW}$	MCL_{GW} = Maximum contaminant level DAF = Groundwater dilution factor

For On-site Receptors DAF = 1

Table 26. SSTL: TPH Mixtures

MADEP CLASSIFICATION

Hydrocarbons C< 12

$$SSTL_{C<12} = \min\left(SSTL_{\mathrm{MADEP1}} / f_1^{C<12}; SSTL_{\mathrm{MADEP2}} / f_2^{C<12}; ....; SSTL_{\mathrm{MADEPn}} / f_n^{C<12}\right)$$

Hydrocarbons C> 12

$$SSTL_{C>12} = \min\left(SSTL_{\mathrm{MADEP1}} / f_1^{C>12}; SSTL_{\mathrm{MADEP2}} / f_2^{C>12}; ....; SSTL_{\mathrm{MADEPn}} / f_n^{C>12}\right)$$

Total Hydrocarbons

$$SSTL_{HC} = \min\left(SSTL_{\mathrm{MADEP1}} / f_1^{HC}; SSTL_{\mathrm{MADEP2}} / f_2^{HC}; ....; SSTL_{\mathrm{MADEPn}} / f_n^{HC}\right)$$

Nomenclature

$SSTL_{\mathrm{MADEPi}}$ = *calculated SSTL for the i-th MADEP class*

$f_i^{C<12}$ *and* $fraz_i^{C>12}$ = *mass fraction of the i-th MADEP class for C>12 and C<12*

f_i^{HC} = *mass fraction of the i-th MADEP class for total hydrocarbons*

TPHWG CLASSIFICATION

Hydrocarbons C< 12

$$SSTL_{C<12} = \min\left(SSTL_{\mathrm{TPH1}} / f_1^{C<12}; SSTL_{\mathrm{TPH2}} / f_2^{C<12}; ....; SSTL_{\mathrm{TPHn}} / f_n^{C<12}\right)$$

Hydrocarbons C> 12

$$SSTL_{C>12} = \min\left(SSTL_{\mathrm{TPH1}} / f_1^{C>12}; SSTL_{\mathrm{TPH2}} / f_2^{C>12}; ....; SSTL_{\mathrm{TPHn}} / f_n^{C>12}\right)$$

Total Hydrocarbons

$$SSTL_{HC} = \min\left(SSTL_{\mathrm{TPH1}} / f_1^{HC}; SSTL_{\mathrm{TPH2}} / f_2^{HC}; ....; SSTL_{\mathrm{TPHn}} / f_n^{HC}\right)$$

Nomenclature

$SSTL_{\mathrm{TPHi}}$ = *calculated SSTL for the i-th TPH class*

$f_i^{C<12}$ *and* $fraz_i^{C>12}$ = *mass fraction of the i-th TPH class for C>12 and C<12*

f_i^{HC} = *mass fraction of the i-th TPHclass for total hydrocarbons*

Table 27. Screening for free phase migration (NAPL)

Vadose zone (ASTM E2081-00)

$$RBSL_{NAPL} = \frac{\theta_w + H\left(\theta_a - \theta_o\right) + \rho_s \cdot K_s}{\rho_s} \cdot S + \frac{\theta_o \cdot \rho_o}{\rho_s} \cdot 10^6 \frac{mg}{kg}$$

Saturated Zone (ASTM E2081-00)

$$RBSL_{NAPL} = \frac{\left(\theta_{e,sat} - \theta_o\right) + \rho_s \cdot K_s}{\rho_s} \cdot S + \frac{\theta_o \cdot \rho_o}{\rho_s} \cdot 10^6 \frac{mg}{kg}$$

Residual phase volume fraction, *θo* (-)

$$\theta_o = \theta_{e,sat} \cdot S_{r,sat} \quad ; \quad \theta_o = \theta_e \cdot S_r$$

Nomenclature

S_r = *Residual phase void fraction, vadose zone (-)*
$S_{r,sat}$ = *Residual phase void fraction, saturated zone (-)*
θ_w = *Volumetric water content (-)*
θ_a = *Volumetric air content (-)*
θ_e = *Effective porosity, unsaturated zone (-)*
$\theta_{e,sat}$ = *Effective porosity, saturated zone (-)*
K_s = *Soil / water partition coefficient (kg/L)*
H = *Henry constant (-)*
ρ_s = *Dry soil bulk density (g/cm^3)*
ρ_o = *Contaminant density (g/cm^3)*

APP. 2B. REFERENCE CONCENTRATIONS

Table 28. Reference Concentration (CR): air

Outdoor Vapors Inhalation
(reference dose method)

$$CR_{AR.InaO} = \min \begin{cases} CR_{canc} = \dfrac{TR}{SF_{Ina} \cdot EM_{InaO} \cdot ADF} \\ CR_{non.canc} = \dfrac{THQ \cdot RfD_{Ina}}{EM_{InaO} \cdot ADF} \end{cases}$$

CR_{canc} = CR carcinogenic cont.
$CR_{non\cdot canc}$ = CR non-carcinogenic cont
TR = Target Risk
THQ = Target Hazard Index
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose – inhalation
EM_{InaO} = Outdoor inhalation rate
ADF = Atmospheric dispersion factor

Outdoor Vapors Inhalation
(reference concentration method)

$$CR_{AR.InaO} = \min \begin{cases} CR_{canc} = \dfrac{TR}{IUR \cdot EC_{InaO} \cdot ADF} \\ CR_{non.canc} = \dfrac{THQ \cdot RfC}{EC_{InaO} \cdot ADF} \end{cases}$$

CR_{canc} = CR carcinogenic cont.
$CR_{non\cdot canc}$ = CR non-carcinogenic cont
TR = Target Risk
THQ = Target Hazard Index
IUR= Inhalation Unit Risk
RfC_{Ina}= Reference concentration
EC_{InaO} = Outdoor inhalation rate
ADF = Atmospheric dispersion factor

Indoor Vapors Inhalation
(reference dose method)

$$CR_{AR.InaI} = \min \begin{cases} CR_{canc} = \dfrac{TR}{SF_{Ina} \cdot EM_{InaI}} \\ CR_{non.canc} = \dfrac{THQ \cdot RfD_{Ina}}{EM_{InaI}} \end{cases}$$

CR_{canc} = CR carcinogenic cont.
$CR_{non\cdot canc}$ = CR non-carcinogenic cont
TR = Target Risk
THQ = Target Hazard Index
SFI_{na} = Slope factor - inhalation
RfD I_{na} = Reference dose – inhalation
EM_{InaI} = Indoor inhalation rate

Indoor Vapors Inhalation
(reference concentration method)

$$CR_{AR.InaI} = \min \begin{cases} CR_{canc} = \dfrac{TR}{IUR \cdot EC_{InaI}} \\ CR_{non.canc} = \dfrac{THQ \cdot RfC}{EC_{InaI}} \end{cases}$$

CR_{canc} = CR carcinogenic cont.
$CR_{non\cdot canc}$ = CR non-carcinogenic cont
TR = Target Risk
THQ = Target Hazard Index
IUR= Inhalation Unit Risk
EC_{InaI} = Indoor inhalation rate

CR air

$$CR_{AR} = \min\left[CR_{AR.InaO}; CR_{AR.InaI}\right]$$

For On-site Receptors ADF = 1

Table 29. Reference Concentration (CR): Flux-chamber

Outdoor Vapors Inhalation $CR_{FC.InaO} = \frac{CR_{AR.InaO}}{\alpha_{FC} \cdot ADF}$	α_{FC} = Outdoor volatilization factor ADF = Atmospheric dispersion factor

For On-site Receptors ADF = 1

Table 30. Reference Concentration (CR): soil-gas

Outdoor Vapors Inhalation $CR_{SG.InaO} = \frac{CR_{AR.InaO}}{\alpha_{samb} \cdot ADF}$	α_{samb} = Outdoor volatilization factor ADF = Atmospheric dispersion factor
Indoor Vapors Inhalation $CR_{SG.InaI} = \frac{CR_{AR.InaI}}{\alpha_{sesp}}$	α_{sesp} = Indoor volatilization factor
CR soil-gas $CR_{SG} = \min\left[CR_{SG.InaO};CR_{SG.InaI}\right]$	

For On-site Receptors ADF = 1

Table 31. Reference Concentration (CR): eluate surface soil

Groundwater Protection $CR_{ELss} = \frac{MCL_{GW} \cdot DAF}{\alpha_{LFss}}$	MCL = Maximum contaminant level α_{LFss} = Leaching factor DAF = Dilution attenuation factor
Water Ingestion $CR_{ELss} = \min\begin{cases} CR_{canc} = \frac{TR \cdot DAF}{SF_{Ing} \cdot EM_{IngW} \cdot \alpha_{LFss}} \\ CR_{non.canc} = \frac{THQ \cdot RfD_{Ing} \cdot DAF}{EM_{IngW} \cdot \alpha_{LFss}} \end{cases}$	CR_{canc} = CR carcinogenic cont. $CR_{non\cdot canc}$ = CR non-carcinogenic cont TR = Target Risk THQ = Target Hazard Index SFI_{ng} = Slope factor - ingestion RfD I_{ng} = Reference dose – ingestion EM_{IngW} = Outdoor ingestion rate α_{LFss} = Leaching factor DAF = Dilution attenuation factor

For On-site Receptors DAF=1

Table 32. Reference Concentration (CR): eluate subsurface soil

Groundwater Protection

$$CR_{ELsp} = \frac{MCL_{GW} \cdot DAF}{\alpha_{LFsp}}$$

MCL = Maximum contaminant level
α_{LFsp} = Leaching factor
DAF = Dilution attenuation factor

Water Ingestion

$$CR_{ELsp} = \min \begin{cases} CR_{canc} = \dfrac{TR \cdot DAF}{SF_{Ing} \cdot EM_{IngW} \cdot \alpha_{LFsp}} \\ CR_{non.canc} = \dfrac{THQ \cdot RfD_{Ing} \cdot DAF}{EM_{IngW} \cdot \alpha_{LFsp}} \end{cases}$$

CR_{canc} = CR carcinogenic cont.
$CR_{non \cdot canc}$ = CR non-carcinogenic cont
TR = Target Risk
THQ = Target Hazard Index
SFI_{ng} = Slope factor - ingestion
RfD I_{ng} = Reference dose – ingestion
EM_{IngW} = Outdoor ingestion rate
α_{LFsp} = Leaching factor
DAF = Dilution attenuation factor

For On-site Receptors DAF=1

APP. 3A. F&T FACTORS (SOIL AND GROUNDWATER)

The fate and transport factors (*FT*) are involved in the indirect exposure assessment or where contaminants can reach targets only through migration and diffusion from the environmental compartment.

For the calculation of transport factors is essential to determine the physical characteristics of the environmental media affected (Vadose zone, groundwater, indoor and outdoor air) and the physico-chemical characteristics of contaminants in order to assess the distribution and dispersion of contaminants.

The fate and transport factors considered in the software are:

From Surface Soil

- VF_{ss}: Outdoor volatilization factor
- VF_{sesp}: Indoor volatilization factor
- *PEF*: Outdoor particulate emission
- PEF_{in}: Indoor particulate emission
- LF_{ss}: Leaching factor

From Subsurface Soil

- VF_{samb} Outdoor volatilization factor
- VF_{sesp}: Indoor volatilization factor
- LF_{sp}: Leaching factor

From Groundwater

- VF_{wamb}: Outdoor volatilization factor
- VF_{wesp}: Indoor volatilization factor
- *DAF*: Groundwater attenuation factor

Air Dispersion

- *ADF*: Air Dispersion Factor

The main assumptions on which are based the equations are:

- The concentration of pollutants in soil is uniformly distributed and constant throughout the entire exposure period;

- Soil is homogeneous and isotropic and incoherent;

- No biodegradation (with the exception of *DAF*) or other mechanisms of degradation / transformation of pollutants.

Table 33. Surface Soil: Outdoor vapor volatilization

$$VF_{ss}\left[\frac{mg/m^{3}{}_{air}}{mg/kg_{soil}}\right] = \min\begin{cases} VF_{ss}(1) = \dfrac{2\cdot W'\cdot\rho_s}{U_{air}\cdot\delta_{air}}BDF_{Vol}\sqrt{\dfrac{D_s^{eff}\cdot H}{\pi\cdot\tau_{outdoor}\cdot(\theta_w+K_s\cdot\rho_s+H\cdot\theta_a)}}\cdot 10^3 \\[2em] VF_{ss}(2) = \dfrac{W'\cdot\rho_s\cdot d}{U_{air}\cdot\delta_{air}\cdot\tau_{outdoor}}\cdot 10^3 \qquad \text{(optional)} \end{cases}$$

Optional check

$$VF_{ss}(1) = \begin{cases} \dfrac{2\cdot W'\cdot\rho_s}{U_{air}\cdot\delta_{air}}BDF_{Vol}\sqrt{\dfrac{D_s^{eff}\cdot H}{\pi\cdot\tau_{outdoor}\cdot(\theta_w+K_s\cdot\rho_s+H\cdot\theta_a)}}\cdot 10^3 & \text{for } L_{s(SS)} = 0 \\[2em] \dfrac{H\cdot\rho_s}{(\theta_w+K_s\cdot\rho_s+H\cdot\theta_a)\cdot\left(1+\dfrac{U_{air}\cdot\delta_{air}\cdot L_{s(SS)}}{D_s^{eff}\cdot W'}\right)}BDF_{Vol}\cdot 10^3 & \text{for } L_{s(SS)} > 0 \end{cases}$$

Nomenclature

d = Thickness of surface soil source (cm)
$L_{s\ (SS)}$ = Depth to surface soil source (cm)
D_s^{eff} = Effective diffusivity in the vadose zone (cm^2/s)
W' = Width of source area parallel to wind direction (cm)
δ_{air} = Ambient air mixing zone height (cm)
U_{air} = Wind speed(cm/s)
$\tau_{outdoor}$ = Averaging time for vapor flux (s)
θ_w = Volumetric water content in the vadose zone (-)
θ_a = Volumetric air content in the vadose zone (-)
θ_e = Effective porosity in the vadose zone (-)
H = Henry's law constant (-)
ρ_s = Soil bulk density (g/cm^3)
BDF_{Vol} = Biodegradation factor (-)

Table 34. Surface Soil: Indoor vapor volatilization

$$VF_{ssesp}\left[\frac{mg/m^3_{air}}{mg/kg_{soil}}\right]=\min\begin{cases}VF_{ssesp}(1)\\ VF_{ssesp}(2)=\dfrac{\rho_s\cdot d}{L_b\cdot ER\cdot\tau_{indoor}}10^3\end{cases}\qquad\text{(optional)}$$

No differential outdoor/indoor pressure (Δp=0)

$$VF_{ssesp}(1)=\frac{\dfrac{H\cdot\rho_s}{(\theta_w+K_s\cdot\rho_s+H\cdot\theta_a)}\cdot\dfrac{D_s^{eff}}{\left(L_{s(SS)}-Z_{crack}\right)\cdot L_b\cdot ER}}{1+\dfrac{D_s^{eff}}{\left(L_{s(SS)}-Z_{crack}\right)\cdot L_b\cdot ER}+\dfrac{D_s^{eff}\,L_{crack}}{D_{crack}^{eff}\cdot\eta\cdot\left(L_{s(SS)}-Z_{crack}\right)}}\cdot BDF_{Vol}\cdot 10^3$$

Differential outdoor/indoor pressure (Δp≠0)

$$VF_{ssesp}(1)=\frac{\dfrac{H\cdot\rho_s}{(\theta_w+K_s\cdot\rho_s+H\cdot\theta_a)}\cdot\dfrac{D_s^{eff}}{\left(L_{s(SS)}-Z_{crack}\right)\cdot L_b\cdot ER}\cdot e^{\xi}}{e^{\xi}+\dfrac{D_s^{eff}}{\left(L_{s(SS)}-Z_{crack}\right)\cdot L_b\cdot ER}+\dfrac{D_s^{eff}\cdot A_b}{Q_s\cdot\left(L_{s(SS)}-Z_{crack}\right)}\cdot\left(e^{\xi}-1\right)}\cdot BDF_{Vol}\cdot 10^3$$

Convective Air Flow Through Foundation Cracks, Q_s (cm^3/s)

$$Q_s=\frac{2\pi\cdot\Delta p\cdot k_v\cdot X_{crack}}{\mu_{air}\cdot\ln\left(\dfrac{2\cdot Z_{crack}\cdot X_{crack}}{A_b\cdot\eta}\right)}\qquad\qquad \xi=\frac{Q_s\cdot L_{crack}}{D_{crack}^{eff}\cdot A_b\cdot\eta}$$

Nomenclature

L_{crack} = *Thickness foundations (cm)*
L_b = *Enclosed space volume/infiltration area ratio (cm)*
Z_{crack} = *Depth to base of enclosed space foundation (cm)*
d = *Thickness of surface soil source (cm)*
$L_{s\,(SS)}$ = *Depth to surface soil source (cm)*
D_s^{eff} = *Effective diffusivity in the vadose zone (cm^2/s)*
D_{crack}^{eff} = *Effective diffusivity in the foundations (cm^2/s)*
τ_{indoor} = *Averaging time for vapor flux (s)*
ER = *Enclosed-space air exchange rate (1/s)*
η = *Areal fraction of cracks in foundations/walls (-)*
θ_w = *Volumetric water content in the vadose zone (-)*
θ_a = *Volumetric air content in the vadose zone (-)*
θ_e = *Effective porosity in the vadose zone (-)*
H = *Henry's law constant (-)*
ρ_s = *Soil bulk density (g/cm^3)*
X_{crack} = *Enclosed space foundation perimeter (cm)*
Δp = *Differential indoor/outdoor air pressure (g/cm^2/s)*
k_v = *Soil vapor permeability (cm^2)*
A_b = *Area of building foundation (cm^2)*
μ_{air} = *Vapor Viscosity (g/cm/s)*
BDF_{Vol} = *Biodegradation factor (-)*

Table 35. Surface Soil: Leaching Factor

$$LF\left[\frac{mg/L_{wat}}{mg/kg_{soil}}\right]=\min\begin{cases}LF(1)=\dfrac{K_{ws}\cdot SAM}{LDF}\cdot BDF_{LF} & \\ LF(2)=\dfrac{d\cdot\rho_s}{I_{eff}\cdot\tau_{LF}} & \text{(optional)}\end{cases}$$

Soil Attenuation model, SAM (-)

$$SAM=\frac{d}{L_{gw}-L_{s(SS)}}\qquad\text{(optional)}$$

Dilution Factor, LDF (-)

$$LDF=1+\frac{v_{gw}\cdot\delta_{gw}}{I_{eff}\cdot W}$$

Partition Coefficient (kg/L)

$$K_{ws}=\frac{\rho_s}{\theta_w+K_s\cdot\rho_s+H\cdot\theta_a}\qquad K_s=\begin{cases}K_d & \text{inorganics}\\ K_{oc}\cdot f_{oc} & \text{organics}\end{cases}$$

Groundwater mixing zone thickness, δ_{gw} *(cm)*

$$\delta_{gw}=(2\cdot 0.0056\cdot W^2)^{0,5}+d_a\cdot\left[1-\exp\left(-\frac{W\cdot I_{eff}}{v_{gw}\cdot d_a}\right)\right]\qquad\text{for }\delta_{gw}>d_a\rightarrow\delta_{gw}=d_a$$

Infiltration Rate (Optional)

$$I_{eff}=\beta\cdot P^2\cdot\eta_{outdoor}$$

Sandy Soils (Sand, Loamy Sand and SandyLoam) β =0.0018; SIlty Soils (Sandy Clay Loam, Loam, Silt Loam and Silt) β =0.0009; Clay Soils (Clay Loam, Silty Clay Loam, Silty Clay, Sandy Clay and Clay) β =0.00018.

Nomenclature

d = Thickness of surface soil source (cm)
L_{gw} *= Depth to groundwater. (cm)*
$L_{s\,(SS)}$ *= Depth to surface soil source (cm)*
v_{gw}*= Groundwater Darcy velocity (cm/s)*
K_{sat}*= Hydraulic Conductivity (cm/s)*
I_{eff} *= Infiltration Rate (cm/s)*
τ_{LF} *= Averaging time for leachate flux (s)*
θ_w *= Volumetric water content in the vadose zone (-)*
θ_a *= Volumetric air content in the vadose zone (-)*
θ_e *= Effective porosity in the vadose zone (-)*
H = Henry's law constant (-)
ρ_s *= Soil bulk density (g/cm*^{3}*)*
f_{oc} *= Organic Carbon Fraction (-)*
d_a *= Groundwater Thickness (cm)*
W = Width of source area parallel to groundwater flow direction (cm)
α_z *= Vertical Dispersivity (cm)*
BDF_{LF} *= Biodegradation factor (-)*

Table 36. Surface Soil: Particulate emission

Outdoor air

$$PEF\left[\frac{mg/m^3{}_{air}}{mg/kg_{soil}}\right]=\frac{P_e\cdot W'}{U_{air}\cdot\delta_{air}}\cdot 10^3$$

Indoor air

$$PEF_{in}\left[\frac{mg/m^3{}_{air}}{mg/kg_{soil}}\right]=PEF\cdot F_i$$

Nomenclature

W' = Width of source area parallel to wind direction (cm)

δ_{air} *= Ambient air mixing zone height (cm)*

U_{air} *= Wind speed(cm/s)*

P_e *= Particulate emission rate (g/cm^2/s)*

Fi = Particulate Indoor fraction (-)

Table 37. Air Dispersion Factor

$$ADF\left[\frac{mg/m^3{}_{air,offsite}}{mg/m^3{}_{air,onsite}}\right]=\frac{Q}{2\pi\cdot U_{air}\cdot\sigma_y\cdot\sigma_z}\cdot\left[2\cdot\exp\left(-\frac{1}{2}\frac{\delta_{air}{}^2}{\sigma_z{}^2}\right)\right]$$

Where Q [cm^3/s]:

$$Q=U_{air}\cdot\delta_{air}\cdot S_w$$

Note that if the calculated ADF value is higher than 1, the ADF is assumed to be equal to the unit value (ADF = 1).

Nomenclature

S_w *= Width of source area orthogonal to wind direction* (cm)

δ_{air} *= Ambient air mixing zone height* (cm)

U_{air} *= Wind Speed (cm/s)*

σ_y *= Transverse air dispersion coefficient* (cm)

σ_z *= Vertical air dispersion coefficient* (cm)

Table 38. Atmospheric Dispersion coefficient

Empirical equations implemented in the software for the determination of dispersion coefficients in the atmosphere (Briggs, 1973).

Stability Class	**σy (m)**	**σz (m)**
Rural Areas		
A	$0.22d\ (1 + 0.0001d)^{-1/2}$	$0.20d$
B	$0.16d\ (1 + 0.0001d)^{-1/2}$	$0.12d$
C	$0.11d\ (1 + 0.0001d)^{-1/2}$	$0.07d\ (1 + 0.0002d)^{-1/2}$
D	$0.08d\ (1 + 0.0001d)^{-1/2}$	$0.06d\ (1 + 0.0015d)^{-1/2}$
E	$0.06d\ (1 + 0.0001d)^{-1/2}$	$0.03d\ (1 + 0.0003d)^{-1}$
F	$0.04d\ (1 + 0.0001d)^{-1/2}$	$0.016d\ (1 + 0.0003d)^{-1}$
Urban Areas		
A – B	$0.32d\ (1 + 0.0004d)^{-1/2}$	$0.24\ (1 + 0.001d)^{-1/2}$
C	$0.22d\ (1 + 0.0004d)^{-1/2}$	$0.20d$
D	$0.16d\ (1 + 0.0004d)^{-1/2}$	$0.14d\ (1 + 0.0003d)^{-1/2}$
E - F	$0.11d\ (1 + 0.0004d)^{-1/2}$	$0.08d\ (1 + 0.00015d)^{-1/2}$

These equations are valid for $100\ m < d < 10000\ m$

Nomenclature
σ_y = *Transverse dispersion coefficient (m)*
σ_z = *Vertical dispersion coefficient (m)*
d = Off-site receptor distance (m)

Table 39. Wind speed at the mixing height

Equation implemented in the software for estimating wind speed at the mixing height (δair)

$$\frac{U_{air}(z_1)}{U_{air}(z_2)} = \left(\frac{z_1}{z_2}\right)^p$$

Empirical coefficient "p"						
Stability Class	**A**	**B**	**C**	**D**	**E**	**F**
Urban Areas	0.15	0.15	0.20	0.25	0.40	0.60
Rural Areas	0.07	0.07	0.10	0.15	0.35	0.55

Table 40. Subsurface Soil: Outdoor vapor volatilization

$$VF_{samb}\left[\frac{mg/m^{3}{}_{air}}{mg/kg_{soil}}\right]=\min\begin{cases} VF_{samb}(1)=\dfrac{H\cdot\rho_s}{(\theta_w+K_s\cdot\rho_s+H\cdot\theta_a)\cdot\left(1+\dfrac{U_{air}\cdot\delta_{air}\cdot L_{s(SP)}}{D_s^{eff}\cdot W'}\right)}\cdot BDF_{Vol}\cdot 10^{3} \\ \\ VF_{samb}(2)=\dfrac{W'\cdot\rho_s\cdot d_s}{U_{air}\cdot\delta_{air}\cdot\tau_{outdoor}}\cdot 10^{3} \qquad \text{(optional)} \end{cases}$$

Nomenclature

d_s= Thickness of subsurface soil source (cm)
$L_{s\ (SP)}$ = Depth to subsurface soil source (cm)
D_s^{eff} = Effective diffusivity in the vadose zone (cm^2/s)
W' = Width of source area parallel to wind direction (cm)
δ_{air} = Ambient air mixing zone height (cm)
U_{air} = Wind speed(cm/s)
$\tau_{outdoor}$ = Averaging time for vapor flux (s)
θ_w = Volumetric water content in the vadose zone (-)
θ_a = Volumetric air content in the vadose zone (-)
θ_e = Effective porosity in the vadose zone (-)
H = Henry's law constant (-)
ρ_s = Soil bulk density (g/cm^3)
BDF_{Vol} = Biodegradation factor (-)

Table 41. Subsurface Soil: Indoor vapor volatilization

$$VF_{sesp}\left[\frac{mg/m^3_{air}}{mg/kg_{soil}}\right] = \min\begin{cases} VF_{sesp}(1) \\ VF_{sesp}(2) = \dfrac{\rho_s \cdot d_s}{L_b \cdot ER \cdot \tau_{indoor}} 10^3 \qquad \text{(optional)} \end{cases}$$

No differential outdoor/indoor pressure (Δp=0)

$$VF_{sesp}(1) = \frac{\dfrac{H \cdot \rho_s}{(\theta_w + K_s \cdot \rho_s + H \cdot \theta_a)} \cdot \dfrac{D_s^{eff}}{\left(L_{s(SP)} - Z_{crack}\right) \cdot L_b \cdot ER}}{1 + \dfrac{D_s^{eff}}{\left(L_{s(SP)} - Z_{crack}\right) \cdot L_b \cdot ER} + \dfrac{D_s^{eff} L_{crack}}{D_{crack}^{eff} \cdot \eta \cdot \left(L_{s(SP)} - Z_{crack}\right)}} \cdot BDF_{Vol} \cdot 10^3$$

Differential outdoor/indoor pressure (Δp≠0)

$$VF_{sesp}(1) = \frac{\dfrac{H \cdot \rho_s}{(\theta_w + K_s \cdot \rho_s + H \cdot \theta_a)} \cdot \dfrac{D_s^{eff}}{\left(L_{s(SP)} - Z_{crack}\right) \cdot L_b \cdot ER} \cdot e^{\xi}}{e^{\xi} + \dfrac{D_s^{eff}}{\left(L_{s(SP)} - Z_{crack}\right) \cdot L_b \cdot ER} + \dfrac{D_s^{eff} \cdot A_b}{Q_s \cdot \left(L_{s(SP)} - Z_{crack}\right)} \cdot \left(e^{\xi} - 1\right)} \cdot BDF_{Vol} \cdot 10^3$$

Convective Air Flow Through Foundation Cracks, Q_s (cm^3/s)

$$Q_s = \frac{2\pi \cdot \Delta p \cdot k_v \cdot X_{crack}}{\mu_{air} \cdot \ln\left(\dfrac{2 \cdot Z_{crack} \cdot X_{crack}}{A_b \cdot \eta}\right)} \qquad \xi = \frac{Q_s \cdot L_{crack}}{D_{crack}^{eff} \cdot A_b \cdot \eta}$$

Nomenclature

L_{crack} = Thickness foundations (cm)
L_b = Enclosed space volume/infiltration area ratio (cm)
Z_{crack} = Depth to base of enclosed space foundation (cm)
d_s = Thickness of subsurface soil source (cm)
$L_{s\,(SP)}$ = Depth to subsurface soil source (cm)
D_s^{eff} = Effective diffusivity in the vadose zone (cm^2/s)
D_{crack}^{eff} = Effective diffusivity in the foundations (cm^2/s)
τ_{indoor} = Averaging time for vapor flux (s)
ER = Enclosed-space air exchange rate (1/s)
η = Areal fraction of cracks in foundations/walls (-)
θ_w = Volumetric water content in the vadose zone (-)
θ_a = Volumetric air content in the vadose zone (-)
θ_e = Effective porosity in the vadose zone (-)
H = Henry's law constant (-)
ρ_s = Soil bulk density (g/cm^3)
X_{crack} = Enclosed space foundation perimeter (cm)
Δp = Differential indoor/outdoor air pressure (g/cm^2/s)
k_v = Soil vapor permeability (cm^2)
A_b = Area of building foundation (cm^2)
μ_{air} = Vapor Viscosity (g/cm/s)
BDF_{Vol} = Biodegradation factor (-)

Table 42. Subsurface Soil: Leaching Factor

$$LF_{sp}\left[\frac{mg/L_{wat}}{mg/kg_{soil}}\right] = \min\begin{cases} LF_{sp}(1) = \dfrac{K_{ws}\cdot SAM}{LDF}\cdot BDF_{LF} & \\ LF_{sp}(2) = \dfrac{d_s\cdot \rho_s}{I_{eff}\cdot \tau_{LF}} & \text{(optional)} \end{cases}$$

Soil Attenuation model, SAM (-)

$$SAM = \frac{d_s}{L_{gw} - L_{s(SP)}} \qquad \text{(optional)}$$

Dilution Factor, LDF (-)

$$LDF = 1 + \frac{v_{gw}\cdot \delta_{gw}}{I_{eff}\cdot W}$$

Partition Coefficient (kg/L)

$$K_{ws} = \frac{\rho_s}{\theta_w + K_s\cdot \rho_s + H\cdot \theta_a} \qquad\qquad K_s = \begin{cases} K_d & \text{inorganics} \\ K_{oc}\cdot f_{oc} & \text{organics} \end{cases}$$

Groundwater mixing zone thickness, δ_{gw} *(cm)*

$$\delta_{gw} = (2\cdot 0.0056\cdot W^2)^{0,5} + d_a\cdot\left[1-\exp\left(-\frac{W\cdot I_{eff}}{v_{gw}\cdot d_a}\right)\right] \qquad \text{for } \delta_{gw} > d_a \;\rightarrow\; \delta_{gw} = d_a$$

Infiltration Rate

$$I_{eff} = \beta\cdot P^2\cdot \eta_{outdoor}$$

Sandy Soils (Sand, Loamy Sand and SandyLoam) β =0.0018; SIlty Soils (Sandy Clay Loam, Loam, Silt Loam and Silt) β =0.0009; Clay Soils (Clay Loam, Silty Clay Loam, Silty Clay, Sandy Clay and Clay) β =0.00018.

Nomenclature

d_s = *Thickness of subsurface soil source (cm)*
L_{gw} = *Depth to groundwater (cm)*
$L_{s\,(SP)}$ = *Depth to subsurface soil source (cm)*
v_{gw}= *Groundwater Darcy velocity (cm/s)*
K_{sat}= *Hydraulic Conductivity (cm/s)*
I_{eff} = *Infiltration Rate (cm/s)*
τ_{LF} = *Averaging time for leachate flux (s)*
θ_w = *Volumetric water content in the vadose zone (-)*
θ_a = *Volumetric air content in the vadose zone (-)*
θ_e = *Effective porosity in the vadose zone (-)*
H = Henry's law constant (-)
ρ_s = *Soil bulk density* (g/cm^3)
f_{oc} = *Organic Carbon Fraction (-)*
d_a = *Groundwater Thickness (cm)*
W = Width of source area parallel to groundwater flow direction (cm)
α_z = *Vertical Dispersivity (cm)*
BDF_{LF} = *Biodegradation factor (-)*

Table 43. Groundwater Attenuation Factor

DAF1 (-)

$$\frac{1}{DAF1}=\exp\left[\frac{x}{2\cdot\alpha_x}\left(1-\sqrt{1+\frac{4\cdot\lambda\cdot\alpha_x\cdot R}{v_e}}\right)\right]\cdot\left[erf\left(\frac{S_w}{4\sqrt{\alpha_y\cdot x}}\right)\right]\cdot\left[erf\left(\frac{\delta_{gw}}{4\sqrt{\alpha_z\cdot x}}\right)\right]$$

DAF2 (-)

$$\frac{1}{DAF2}=\exp\left[\frac{x}{2\cdot\alpha_x}\left(1-\sqrt{1+\frac{4\cdot\lambda\cdot\alpha_x\cdot R}{v_e}}\right)\right]\cdot\left[erf\left(\frac{S_w}{4\sqrt{\alpha_y\cdot x}}\right)\right]\cdot\left[erf\left(\frac{\delta_{gw}}{2\sqrt{\alpha_z\cdot x}}\right)\right]$$

DAF3(-)

$$\frac{1}{DAF3}=\exp\left[\frac{x}{2\cdot\alpha_x}\left(1-\sqrt{1+\frac{4\cdot\lambda\cdot\alpha_x\cdot R}{v_e}}\right)\right]\cdot\left[erf\left(\frac{S_w}{4\sqrt{\alpha_y\cdot x}}\right)\right]$$

Effective groundwater velocity, v_e (cm/s)

$$v_e=\frac{K_{sat}\cdot i}{\theta_{e,sat}}$$

Constituent retardation factor, R (-)

$$R=1+K_s\frac{\rho_s}{\theta_{e,sat}}$$

Longitudinal Dispersivity, α_x (cm)

$$\alpha_x=POC/10$$

Transversal Dispersivity, α_y (cm)

$$\alpha_y=\alpha_x/3$$

Vertical Dispersivity, α_z (cm)

$$\alpha_z=\alpha_x/20$$

Nomenclature

λ = First-order degradation rate (1/s)
S_w = Width of source area orthogonal to groundwater flow (cm)
δ_{gw} = Groundwater mixing zone thickness (cm)
x = distance(cm)
K_s = Soil-water sorption coefficient (mg/kg/mg/L)
$\theta_{e,sat}$ = Effective porosity, saturated zone (-)
ρ_s = Soil bulk density (g/cm^3)
i = Hydraulic gradient (-)
K_{sat} = Hydraulic conductivity(cm/s)
POC = Distance to groundwater receptor (cm)

Table 44. Groundwater: Indoor Vapors Volatilization

No differential outdoor/indoor pressure (Δp=0)

$$VF_{wesp}\left[\frac{mg/m^{3}{}_{air}}{mg/L_{water}}\right]=\frac{H\cdot\frac{D_{w}^{eff}}{\left(L_{gw}-Z_{crack}\right)L_{b}\cdot ER}}{1+\frac{D_{w}^{eff}}{\left(L_{gw}-Z_{crack}\right)L_{b}\cdot ER}+\frac{D_{w}^{eff}\cdot L_{crack}}{D_{crack}^{eff}\left(L_{gw}-Z_{crack}\right)\eta}}\cdot BDF_{Vol}\cdot 10^{3}$$

Differential outdoor/indoor pressure (Δp=0)

$$VF_{wesp}\left[\frac{mg/m^{3}{}_{air}}{mg/L_{water}}\right]=\frac{H\cdot\frac{D_{w}^{eff}}{\left(L_{gw}-Z_{crack}\right)L_{b}\cdot ER}\cdot e^{\xi}}{e^{\xi}+\frac{D_{w}^{eff}}{\left(L_{gw}-Z_{crack}\right)L_{b}\cdot ER}+\frac{D_{w}^{eff}\cdot A_{b}}{Q_{s}\cdot\left(L_{gw}-Z_{crack}\right)}\cdot\left(e^{\xi}-1\right)}\cdot BDF_{Vol}\cdot 10^{3}$$

Convective Air Flow Through Foundation Cracks, Q_s (cm^3/s)

$$Q_{s}=\frac{2\pi\cdot\Delta p\cdot k_{v}\cdot X_{crack}}{\mu_{air}\cdot\ln\left(\frac{2\cdot Z_{crack}\cdot X_{crack}}{A_{b}\cdot\eta}\right)}\qquad\qquad \xi=\frac{Q_{s}\cdot L_{crack}}{D_{crack}^{eff}\cdot A_{b}\cdot\eta}$$

Nomenclature

L_{crack} = *Thickness foundations (cm)*
L_b = *Enclosed space volume/infiltration area ratio (cm)*
Z_{crack} = *Depth to base of enclosed space foundation (cm)*
L_{gw} = *Depth to groundwater (cm)*
D_w^{eff} = *Effective diffusivity from groundwater* (cm^2/s)
D_{crack}^{eff} = *Effective diffusivity in the foundations* (cm^2/s)
τ_{indoor} = *Averaging time for vapor flux (s)*
ER = Enclosed-space air exchange rate (1/s)
η = *Areal fraction of cracks in foundations/walls (-)*
θ_w = *Volumetric water content in the vadose zone (-)*
θ_a = *Volumetric air content in the vadose zone (-)*
θ_e = *Effective porosity in the vadose zone (-)*
H = Henry's law constant (-)
ρ_s = *Soil bulk density* (g/cm^3)
X_{crack} = *Enclosed space foundation perimeter (cm)*
Δp = *Differential indoor/outdoor air pressure* ($g/cm^2/s$)
k_v = *Soil vapor permeability* (cm^2)
A_b = *Area of building foundation* (cm^2)
μ_{air} = *Vapor Viscosity (g/cm/s)*
BDF_{Vol} = *Biodegradation factor (-)*

Table 45. Groundwater: Outdoor Vapors Volatilization

$$VF_{wamb}\left[\frac{mg/m^{3}{}_{air}}{mg/L_{wat}}\right]=\frac{H}{1+\dfrac{U_{air}\cdot\delta_{air}\cdot L_{gw}}{D_{w}^{eff}\cdot W'}}\cdot BDF_{Vol}\cdot 10^{3}$$

Nomenclature

L_{gw}= Depth to Groundwater cm)
D_w^{eff}= Effective diffusivity from groundwater (cm^2/s)
W' = Width of source area parallel to wind direction (cm)
δ_{air} = Ambient air mixing zone height (cm)
U_{air} = Wind speed(cm/s)
H = Henry's law constant (-)
BDF_{Vol} = Biodegradation factor (-)

Table 46. Diffusion Coefficient

Diffusion Coefficient in the vadose zone

$$D_s^{eff}\left[\frac{cm^2}{s}\right]=\frac{D_a\cdot\theta_a^{\;3,33}}{\theta_e^{\;2}}+\frac{D_w\cdot\theta_w^{\;3,33}}{H\cdot\theta_e^{\;2}}$$

Diffusion Coefficient in the capillary fringe

$$D_{cap}^{eff}\left[\frac{cm^2}{s}\right]=\frac{D_a\cdot\theta_{acap}^{\;3,33}}{\theta_{e,cap}^{\;2}}+\frac{D_w\cdot\theta_{wcap}^{\;3,33}}{H\cdot\theta_{e,cap}^{\;2}}$$

Diffusion Coefficient in the clay lens

$$D_{lente}^{eff}\left[\frac{cm^2}{s}\right]=\frac{D_a\cdot\theta_{alens}^{\;3,33}}{\theta_{e,lens}^{\;2}}+\frac{D_w\cdot\theta_{wlens}^{\;3,33}}{H\cdot\theta_{e,lens}^{\;2}}$$

Diffusion Coefficient in the foundations

$$D_{crack}^{eff}\left[\frac{cm^2}{s}\right]=\frac{D_a\cdot\theta_{acrack}^{\;3,33}}{\theta_{e,crack}^{\;2}}+\frac{D_w\cdot\theta_{wcrack}^{\;3,33}}{H\cdot\theta_{e,crack}^{\;2}}$$

Diffusion Coefficient from groundwater

$$D_w^{eff}\left[\frac{cm^2}{s}\right]=\frac{h_{cap}+h_v}{\dfrac{h_{cap}}{D_{cap}^{eff}}+\dfrac{h_v}{D_s^{eff}}}$$

Diffusion Coefficient in the presence of a clay lens

$$D_{s+lente}^{eff}\left[\frac{cm^2}{s}\right]=\frac{L_s}{\dfrac{L_s-d_{lens}}{D_{suolo}^{eff}}+\dfrac{d_{lens}}{D_{lente}^{eff}}}$$

Nomenclature

h_{cap} = *Capillary fringe thickness (cm)*
h_v = *Vadose zone thickness (cm)*
d_{lens} = *Thickness of the lens (cm)*
D_a = *Diffusion coefficient in air* (cm^2/s)
D_w = *Diffusion coefficient in water* (cm^2/s)
θ_w = *Volumetric water content in the vadose zone (-)*
θ_a = *Volumetric air content in the vadose zone (-)*
θ_{wcap} = *Volumetric water content in the capillary fringe (-)*
θ_{acap} = *Volumetric air content in the capillary fringe (-)*
θ_{wlens} = *Volumetric water content in the lens (-)*
θ_{alens} = *Volumetric air content in the lens (-)*
θ_{wcrack} = *Volumetric water content in the foundations (-)*
θ_{acrack} = *Volumetric air content in the foundations (-)*
θ_e = *Effective Porosity in the vadose zone (-)*
$\theta_{e,cap}$ = *Effective Porosity in the capillary fringe (-)*
$\theta_{e,crack}$ = *Effective Porosity in the foundations (-)*
H = *Henry's law constant (-)*
ρ_s = *Soil bulk density* (g/cm^3)

Table 47. Saturation Concentration (C_{sat})

Saturation Concentration

$$C_{sat}\left[mg/kg\right]=\frac{\theta_w+H\cdot\theta_a+\rho_s\cdot K_s}{\rho_s}\cdot S$$

Nomenclature

θ_w = *Volumetric water content in the vadose zone (-)*
θ_a = *Volumetric air content in the vadose zone (-)*
S = *Solubility (mg/L)*
H = *Henry's law constant (-)*
ρ_s = *Soil bulk density (g/cm^3)*

Table 48. Biodegradation factor (BDF) per the volatilization pathway

Biodegradation factor (optional) is valid only for L_s >0 *(Source: Verginelli and Baciocchi, 2014)*
Outdoor volatilization

$$BDF_{Vol} = 2 \cdot \frac{\exp(-kL_a)}{1 + k\left(L_s - L_a\right)} \qquad \text{con} \qquad k = \sqrt{\frac{\lambda \cdot \theta_w}{H \cdot D_s^{eff}}}$$

Nomenclature
L_s = *Depth of the source (cm) **
L_a = *Depth of the aerobic zone (cm)*
D_s^{eff} = *Effective diffusivity in the vadose zone (cm²/s)*
θ_w = *Volumetric water content in the vadose zone (-)*
H = Henry's law constant (-)
λ = First-order biodegradation constant (1/s)

Biodegradation factor (optional) is valid only for $L_s - Z_{crack}$ >0 *(Source: Verginelli and Baciocchi, 2014)*

Outdoor volatilization

$$BDF_{Vol} = 2 \cdot \frac{\exp(-kL_{a,indoor})}{1 + k\left(L_s - Z_{crack} - L_{a,indoor}\right)} \qquad \text{with} \qquad k = \sqrt{\frac{\lambda \cdot \theta_w}{H \cdot D_s^{eff}}}$$

Nomenclature
L_s = *Depth of the source (cm) **
D_s^{eff} = *Effective diffusivity in the vadose zone (cm²/s)*
θ_w = *Volumetric water content in the vadose zone (-)*
H = Henry's law constant (-)
Z_{crack} = *Depth to the base of enclosed space foundation (cm)*
$L_{a,indoor}$ = *Depth of the aerobic zone from building foundations (cm)*
λ = First-order biodegradation constant (1/s)

** For soil-gas data L_s is the depth of the probe*

Table 49. Biodegradation factor (BDF) per the leaching pathway

Biodegradation factor (BDF) per the leaching pathway *(Source: Green Ampt)*

$$BDF_{LF} = \exp\left[-\left(\frac{\lambda \cdot R}{v_{gw}} \right) \cdot L \right]$$

Time to reach the water table, t_{gw} (cm/s)

$$t_{gw} = \frac{\theta_a}{K_{sat}} \cdot \left[L - \left(H_w - h_{cr} \right) \cdot \ln\left(\frac{H_w + L - h_{cr}}{H_w - h_{cr}} \right) \right]$$

Water infiltration velocity, v_{gw} (cm/s)

$$v_{gw} = \frac{L}{t_{gw}}$$

Infiltration velocity of the contaminant v_c (cm/s)

$$v_c = \frac{v_{gw}}{R}$$

Retardation factor, R (-)

$$R = 1 + K_s \frac{\rho_s}{\theta_e}$$

Nomenclature

λ = First-order biodegradation constant (1/s)
H_w = Ponding depth (cm)
L = Depth of the water table from the bottom of the source (cm)
hcr = Wetting front suction (matric potential) (cm)
$\theta_{e,}$ = Effective porosity in the unsaturated zone (-)
K_s = Partition Coefficient (mg/kg/mg/L)
ρ_s = Soil bulk density (g/cm^3)
K_{sat} = Hydraulic conductivity in the vadose zone (cm/s)

Table 50. Infiltration Rate

Infiltration Rate

$$I_{eff} = \beta \cdot P^2 \cdot \eta_{outdoor}$$

Sandy Soils (Sand, Loamy Sand and SandyLoam) β =0.0018; SIlty Soils (Sandy Clay Loam, Loam, Silt Loam and Silt) β =0.0009; Clay Soils (Clay Loam, Silty Clay Loam, Silty Clay, Sandy Clay and Clay) β =0.00018.

Effective infiltration in the presence of a low permeability layer between the source and the water table (ISPRA, 2005)

$$I_{eff} = K_{unsat} \cdot i_f$$

Vertical hydraulic gradient

$$i_f = \frac{h_{perc} + d_{unsat}}{d_{unsat}}$$

Effective infiltration in the presence of a HDPE sheet (ISPRA, 2005)

$$I_{eff} = \rho_m \cdot L'_{fm} + \rho_f \cdot L'_{ff} + \rho_s \cdot L'_{fs}$$

where:

$$\begin{cases} L'_{fm} = C_d \cdot i_{av} \cdot h_{perc}^{\,0.9} \cdot a_m^{\,0.1} \cdot K_{eq}^{\,0.74} & \text{cracks} \\ L'_{ff} = C_d \cdot i_{av} \cdot h_{perc}^{\,0.9} \cdot a_f^{\,0.1} \cdot K_{eq}^{\,0.74} & \text{holes} \\ L'_{fs} = C_d \cdot i_{av} \cdot h_{perc}^{\,0.9} \cdot a_s^{\,0.1} \cdot K_{eq}^{\,0.74} & \text{patches} \end{cases}$$

Vertical hydraulic gradient

$$i_{av} = 1 + 0{,}1 \cdot \left(\frac{h_{perc}}{d_{unsat}} \right)^{0{,}95}$$

Nomenclature

a_m, a_f, a_s: Cracks, holes and patches area in the HDPE sheet (cm^2)

C_d: Empirical constant for the quality of the contact of the HDPE sheet (-)

d_{unsat}: Thickness of the low-permeability layer (below the HDPE sheet if present) (cm)

h_{perc}: Hydraulic head above the HDPE sheet or the low-permeability layer (cm)

i_{av}: Vertical hydraulic gradient (-)

K_{unsat} : Hydraulic conductivity of the low-permeability layer (below HDPE if present) (cm/y)

ρ_m, ρ_f, ρ_s: Cracks, holes and patches density in the HDPE sheet (#/cm^2)

P = rainfall (cm/y)

APP. 3B. F&T FACTORS (BACKFILL MATERIALS)

The fate and transport factors considered in the software for Backfill Materials are:

- VF_{MdR}: Outdoor volatilization factor
- $VF_{MdR,esp}$ Indoor volatilization factor
- PEF_{MdR}: Outdoor particulate emission
- $PEF_{MdtR,in}$: Indoor particulate emission
- LF_{MdR}: Leaching factor

Air Dispersion

- *ADF*: Air Dispersion Factor

Table 51. Backfill Material: Outdoor vapor volatilization

$$VF_{MdR}\left[\frac{mg/m^{3}{}_{air}}{mg/kg_{soil}}\right]=\min\begin{cases} VF_{MdR}(1)=\dfrac{2\cdot W'_{MdR}\cdot\rho_{MdR}}{U_{air}\cdot\delta_{air}}BDF_{Vol}\sqrt{\dfrac{D^{eff}_{MdR}\cdot H}{\pi\cdot\tau_{outdoor}\cdot(\theta_{w,\mathrm{MdR}}+K_{s,MdR}\cdot\rho_{MdR}+H\cdot\theta_{a,\mathrm{MdR}})}}\cdot 10^{3} \\ VF_{MdR}(2)=\dfrac{W'\cdot\rho_{MdR}\cdot d_{MdR}}{U_{air}\cdot\delta_{air}\cdot\tau_{outdoor}}\cdot 10^{3} \qquad \text{(optional)} \end{cases}$$

Optional check

$$VF_{MdR}(1)=\begin{cases} \dfrac{2\cdot W'_{MdR}\cdot\rho_{MdR}}{U_{air}\cdot\delta_{air}}BDF_{Vol}\sqrt{\dfrac{D^{eff}_{MdR}\cdot H}{\pi\cdot\tau_{outdoor}\cdot(\theta_{w,MdR}+K_{s,MdR}\cdot\rho_{MdR}+H\cdot\theta_{a,MdR})}}\cdot 10^{3} & \text{if } L_{MdR}=0 \\ \dfrac{H\cdot\rho_{s}}{(\theta_{w,MdR}+K_{s,MdR}\cdot\rho_{MdR}+H\cdot\theta_{a,MdR})\cdot\left(1+\dfrac{U_{air}\cdot\delta_{air}\cdot L_{MdR}}{D^{eff}_{MdR}\cdot W'}\right)}BDF_{Vol}\cdot 10^{3} & \text{if } L_{MdR}>0 \end{cases}$$

Nomenclature

d_{MdR} = *Thickness of backfill material (cm)*
L_{MdR} = *Depth to backfill material (cm)*
D_{MdR}^{ef} = *Effective diffusivity in the backfill material (cm^2/s)*
W' = Width of source area parallel to wind direction (cm)
δ_{air} = *Ambient air mixing zone height (cm)*
U_{air} = *Wind speed(cm/s)*
$\tau_{outdoor}$ = *Averaging time for vapor flux (s)*
$\theta_{w,MdR}$ = *Volumetric water content in the backfill material (-)*
$\theta_{a,MdR}$ = *Volumetric air content in the backfill material (-)*
$\theta_{e,MdR}$ = *Effective porosity in the backfill material (-)*
H = Henry's law constant (-)
ρ_{MdR} = *Bulk density of backfill material (g/cm^3)*
BDF_{Vol} = *Biodegradation factor (-)*

Table 52. Backfill Material: Indoor vapor volatilization

$$VF_{MdR,esp}\left[\frac{mg/m^{3}{}_{air}}{mg/kg_{soil}}\right]=\min\begin{cases}VF_{MdR,esp}(1)\\ VF_{MdR,esp}(2)=\dfrac{\rho_{MdR}\cdot d_{MdR}}{L_{b}\cdot ER\cdot\tau_{indoor}}10^{3}\qquad\text{(optional)}\end{cases}$$

No differential outdoor/indoor pressure (Δp=0)

$$VF_{MdR,esp}(1)=\frac{\dfrac{H\cdot\rho_{MdR}}{(\theta_{w,MdR}+K_{s,MdR}\cdot\rho_{MdR}+H\cdot\theta_{a,MdR})}\cdot\dfrac{D_{MdR}^{eff}}{\left(L_{MdR}-Z_{crack}\right)\cdot L_{b}\cdot ER}}{1+\dfrac{D_{MdR}^{eff}}{\left(L_{MdR}-Z_{crack}\right)\cdot L_{b}\cdot ER}+\dfrac{D_{MdR}^{eff}L_{crack}}{D_{crack}^{eff}\cdot\eta\cdot\left(L_{MdR}-Z_{crack}\right)}}BDF_{Vol}\cdot10^{3}$$

Differential outdoor/indoor pressure (Δp≠0)

$$VF_{MdR,esp}(1)=\frac{\dfrac{H\cdot\rho_{MdR}}{(\theta_{w.MdR}+K_{s.MdR}\cdot\rho_{MdR}+H\cdot\theta_{a.MdR})}\cdot\dfrac{D_{MdR}^{eff}}{\left(L_{MdR}-Z_{crack}\right)\cdot L_{b}\cdot ER}\cdot e^{\xi}}{e^{\xi}+\dfrac{D_{MdR}^{eff}}{\left(L_{MdR}-Z_{crack}\right)\cdot L_{b}\cdot ER}+\dfrac{D_{MdR}^{eff}\cdot A_{b}}{Q_{s}\cdot\left(L_{MdR}-Z_{crack}\right)}\cdot\left(e^{\xi}-1\right)}BDF_{Vol}\cdot10^{3}$$

Convective Air Flow Through Foundation Cracks, Q_s (cm^3/s)

$$Q_{s}=\frac{2\pi\cdot\Delta p\cdot k_{v}\cdot X_{crack}}{\mu_{air}\cdot\ln\left(\dfrac{2\cdot Z_{crack}\cdot X_{crack}}{A_{b}\cdot\eta}\right)}\qquad\qquad \xi=\frac{Q_{s}\cdot L_{crack}}{D_{crack}^{eff}\cdot A_{b}\cdot\eta}$$

Nomenclature

d_{MdR} = Thickness of backfill material (cm)
L_{MdR} = Depth to backfill material (cm)
H = Henry's law constant (-)
ρ_{MdR} = Bulk density of backfill material (g/cm^3)
L_{crack} = Thickness foundations (cm)
L_b = Enclosed space volume/infiltration area ratio (cm)
Z_{crack} = Depth to base of enclosed space foundation (cm)
D_{crack}^{eff} = Effective diffusivity in the foundations (cm^2/s)
D_{MdR}^{ef} = Effective diffusivity in the backfill material (cm^2/s)
$\theta_{w,MdR}$ = Volumetric water content in the backfill material (-)
$\theta_{a,MdR}$ = Volumetric air content in the backfill material (-)
$\theta_{e,MdR}$ = Effective porosity in the backfill material (-)
τ_{indoor} = Averaging time for vapor flux (s)
ER = Enclosed-space air exchange rate (1/s)
η = Areal fraction of cracks in foundations/walls (-)
H = Henry's law constant (-)
X_{crack} = Enclosed space foundation perimeter (cm)
Δp = Differential indoor/outdoor air pressure ($g/cm^2/s$)
k_v = Soil vapor permeability (cm^2)
A_b = Area of building foundation (cm^2)
μ_{air} = Vapor Viscosity (g/cm/s)
BDF_{Vol} = Biodegradation factor (-)

Table 53. Backfill Material: Particulate emission

Outdoor

$$PEF_{MdR}\left[\frac{mg/m^{3}{}_{air}}{mg/kg_{soil}}\right]=\frac{P_{e}\cdot W'}{U_{air}\cdot\delta_{air}}\cdot 10^{3}$$

Indoor

$$PEF_{MdR,in}\left[\frac{mg/m^{3}{}_{air}}{mg/kg_{soil}}\right]=PEF\cdot F_{i}$$

Nomenclature

W' = Width of source area parallel to wind direction (cm)

δ_{air} = *Ambient air mixing zone height (cm)*

U_{air} = *Wind speed(cm/s)*

P_e = *Particulate emission rate (g/cm^2/s)*

Fi = Particulate Indoor fraction (-)

Table 54. Backfill Material: Air Dispersion Factor

$$ADF\left[\frac{mg/m^{3}{}_{air,offsite}}{mg/m^{3}{}_{air,onsite}}\right]=\frac{Q}{2\pi\cdot U_{air}\cdot\sigma_{y}\cdot\sigma_{z}}\cdot\left[2\cdot\exp\left(-\frac{1}{2}\frac{\delta_{air}{}^{2}}{\sigma_{z}{}^{2}}\right)\right]$$

Where Q [cm^3/s]:

$$Q=U_{air}\cdot\delta_{air}\cdot S_{w}$$

Note that if the calculated ADF value is higher than 1, the ADF is assumed to be equal to the unit value (ADF = 1).

Nomenclature

S_w = *Width of source area orthogonal to wind direction* (cm)

δ_{air} = *Ambient air mixing zone height* (cm)

U_{air} = *Wind Speed (cm/s)*

σ_y = *Transverse air dispersion coefficient* (cm)

σ_z = *Vertical air dispersion coefficient* (cm)

Table 55. Backfill Material: Leaching Factor

$$LF_{MdR}\left[\frac{mg/L_{water}}{mg/kg_{soil}}\right]=\min\begin{cases}LF_{MdR}(1)=\dfrac{K_{ws,MdR}\cdot SAM_{\text{mod}}}{LDF}BDF_{LF}\\[2ex] LF_{MdR}(2)=\dfrac{d_{MdR}\cdot\rho_{MdR}}{I_{eff}\cdot\tau_{LF}} \qquad \text{(optional)}\end{cases}$$

Modified Soil Attenuation model, SAM$_{\text{mod}}$ (-)

$$SAM_{\text{mod}}=\frac{d_{MdR}}{d_{MdR}+\left(\dfrac{\theta_w+K_s\cdot\rho_s+H\cdot\theta_a}{\theta_{w,MdR}+K_{s,MdR}\cdot\rho_{MdR}+H\cdot\theta_{a,MdR}}\right)\left(L_{gw}-L_{MdR}-d_{MdR}\right)} \qquad \text{(optional)}$$

Leachate Dilution Factor, LDF (-)

$$LDF=1+\frac{v_{gw}\cdot\delta_{gw}}{I_{eff,MdR}\cdot W}$$

Partition coefficients (kg/L)

$$K_{ws,MdR}=\frac{\rho_{MdR}}{\theta_{w,MdR}+K_{s,MdR}\cdot\rho_{MdR}+H\cdot\theta_{a,MdR}} \qquad K_{s,MdR}=\begin{cases}K_{d,MdR} & \text{inorganics}\\ K_{oc}\cdot f_{oc,MdR} & \text{organics}\end{cases}$$

Groundwater mixing zone thickness, *δ_{gw} (cm)*

$$\delta_{gw}=(2\cdot 0.0056\cdot W^2)^{0,5}+d_a\cdot\left[1-\exp\left(-\frac{W\cdot I_{eff,MdR}}{v_{gw}\cdot d_a}\right)\right] \qquad \text{Se }\delta_{gw}>d_a\ \rightarrow\ \delta_{gw}=d_a$$

Nomenclature

d_{MdR} = Thickness of backfill materials (cm)
L_{gw} = Depth to groundwater. (cm)
L_{MdR} = Depth to backfill materials (cm)
v_{gw}= Groundwater Darcy velocity (cm/s)
K_{sat}= Hydraulic Conductivity (cm/s)
I_{eff} = Infiltration Rate (cm/s)
τ_{LF} = Averaging time for leachate flux (s)
$\theta_{w,MdR}$ = Volumetric water content in the backfill material (-)
$\theta_{a,MdR}$ = Volumetric air content in the backfill material (-)
$\theta_{e,MdR}$ = Effective porosity in the backfill material (-)
H = Henry's law constant (-)
ρ_{MdR} = Bulk density of backfill material (g/cm^3)
f_{oc} = Organic Carbon Fraction (-)
d_a = Groundwater Thickckness (cm)
W = Width of source area parallel to groundwater flow direction (cm)
α_z = Vertical Dispersivity (cm)
BDF_{LF} = Biodegradation factor (-)

Table 56. Backfill Materials: Diffusion Coefficient

Diffusion Coefficient in the backfill materials

$$D_{MdR}^{eff}\left[\frac{cm^2}{s}\right]=\frac{D_a\cdot\theta_{a,MdR}{}^{3,33}}{\theta_{e,MdR}{}^{2}}+\frac{D_w\cdot\theta_{w,MdR}{}^{3,33}}{H\cdot\theta_{e,MdR}{}^{2}}$$

Nomenclature

D_a = Diffusion coefficient in air (cm^2/s)
D_w = Diffusion coefficient in water (cm^2/s)
$\theta_{w,MdR}$ = Volumetric water content in the backfill material (-)
$\theta_{a,MdR}$ = Volumetric air content in the backfill material (-)
$\theta_{e,MdR}$ = Effective porosity in the backfill material (-)
H = Henry's law constant (-)

Table 57. Backfill Materials: Saturation concentration

Saturation concentration

$$C_{sat,MdR}\left[mg/kg\right]=\frac{\theta_{w,MdR}+H\cdot\theta_{a,MdR}+\rho_{MdR}\cdot K_{s,MdR}}{\rho_{MdR}}\cdot S$$

Partition coefficient (kg/L)

$$K_{s,MdR}=\begin{cases}K_{d,MdR} & \text{inorganics}\\ K_{oc}\cdot f_{oc,MdR} & \text{organics}\end{cases}$$

Nomenclatura

$\theta_{w,MdR}$ = Volumetric water content in the backfill material (-)
$\theta_{a,MdR}$ = Volumetric air content in the backfill material (-)
ρ_{MdR} = Bulk density of backfill material (g/cm^3)
f_{oc} = Organic Carbon Fraction (-)
S = solubility (mg/L)
H = Henry's law constant (-)

Table 58. Eluate Backfill Materials: Leachate

$$\alpha_{LF,MdR}\left[\frac{mg/L_{water}}{mg/L_{eluate}}\right]=\frac{SAM_{\mathrm{mod}}}{LDF}\,BDF_{LF}$$

Modified Soil Attenuation model, SAM$_{\mathrm{mod}}$ (-)

$$SAM_{\mathrm{mod}}=\frac{d_{MdR}}{d_{MdR}+\left(\dfrac{\theta_w+K_s\cdot\rho_s+H\cdot\theta_a}{\theta_{w,MdR}+K_{s,MdR}\cdot\rho_{MdR}+H\cdot\theta_{a,MdR}}\right)\left(L_{gw}-L_{MdR}-d_{MdR}\right)}\qquad\text{(optional)}$$

Leachate Dilution Factor, LDF (-)

$$LDF=1+\frac{v_{gw}\cdot\delta_{gw}}{I_{eff,MdR}\cdot W}$$

Groundwater mixing zone thickness, *δ$_{gw}$ (cm)*

$$\delta_{gw}=(2\cdot 0.0056\cdot W^2)^{0,5}+d_a\cdot\left[1-\exp\left(-\frac{W\cdot I_{eff}}{v_{gw}\cdot d_a}\right)\right]\qquad \text{Se }\delta_{gw}>d_a\ \rightarrow\ \delta_{gw}=\ d_a$$

Nomenclature

d_{MdR} = Thickness of backfill materials (cm)
L_{gw} = Depth to groundwater. (cm)
L_{MdR} = Depth to backfill materials (cm)
v_{gw}= Groundwater Darcy velocity (cm/s)
K_{sat}= Hydraulic Conductivity (cm/s)
I_{eff} = Infiltration Rate (cm/s)
τ_{LF} = Averaging time for leachate flux (s)
$\theta_{w,MdR}$ = Volumetric water content in the backfill material (-)
$\theta_{a,MdR}$ = Volumetric air content in the backfill material (-)
$\theta_{e,MdR}$ = Effective porosity in the backfill material (-)
H = Henry's law constant (-)
ρ_{MdR} = Bulk density of backfill material (g/cm^3)
f_{oc} = Organic Carbon Fraction (-)
d_a = Groundwater Thickckness (cm)
W = Width of source area parallel to groundwater flow direction (cm)
α_z = Vertical Dispersivity (cm)
BDF_{LF} = Biodegradation factor (-)

Table 59. Eluate Backfill Materials: pH

pH values due to leaching and dilution of eluate in groundwater

$$[H^+] = \frac{10^{-pH} \cdot 1.01}{1000}$$

$$[H^+]_{out} = \frac{I_{eff,MdR} \cdot W}{I_{eff,MdR} \cdot W + v_{gw} \cdot \delta_{gw}} \cdot SAM_{\mathrm{mod}} \cdot [H^+]_{eluate} + \frac{v_{gw} \cdot \delta_{gw}}{I_{eff,MdR} \cdot W + v_{gw} \cdot \delta_{gw}} \cdot [H^+]_{groundwater}$$

$$pH_{out} = -\log\left(\frac{\left[H^+\right]_{out} \cdot 1000}{1.01}\right)$$

Modified Soil Attenuation model, SAM$_{\mathbf{mod}}$ (-)

$$SAM_{\mathrm{mod}} = \frac{d_{MdR}}{d_{MdR} + \left(\frac{\theta_w + K_s \cdot \rho_s + H \cdot \theta_a}{\theta_{w,MdR} + K_{s,MdR} \cdot \rho_{MdR} + H \cdot \theta_{a,MdR}}\right)\left(L_{gw} - L_{MdR} - d_{MdR}\right)} \qquad \text{(optional)}$$

Nomenclature

d_{MdR} = Thickness of backfill materials (cm)
L_{gw} = Depth to groundwater. (cm)
L_{MdR} = Depth to backfill materials (cm)
v_{gw}= Groundwater Darcy velocity (cm/s)
K_{sat}= Hydraulic Conductivity (cm/s)
I_{eff} = Infiltration Rate (cm/s)
τ_{LF} = Averaging time for leachate flux (s)
$\theta_{w,MdR}$ = Volumetric water content in the backfill material (-)
$\theta_{a,MdR}$ = Volumetric air content in the backfill material (-)
$\theta_{e,MdR}$ = Effective porosity in the backfill material (-)
H = Henry's law constant (-)
ρ_{MdR} = Bulk density of backfill material (g/cm^3)
f_{oc} = Organic Carbon Fraction (-)
d_a = Groundwater Thickckness (cm)
W = Width of source area parallel to groundwater flow direction (cm)
α_z = Vertical Dispersivity (cm)
BDF_{LF} = Biodegradation factor (-)

Tabella 1. COD MdR: Lisciviazione in falda

COD values due to leaching and dilution of eluate in groundwater

$$COD_{out} = \frac{I_{eff,MdR} \cdot W}{I_{eff,MdR} \cdot W + v_{gw} \cdot \delta_{gw}} \cdot SAM_{\mathrm{mod}} \cdot COD_{eluate} + \frac{v_{gw} \cdot \delta_{gw}}{I_{eff,MdR} \cdot W + v_{gw} \cdot \delta_{gw}} \cdot COD_{groundwater}$$

Modified Soil Attenuation model, SAM_{mod} (-)

$$SAM_{\mathrm{mod}} = \frac{d_{MdR}}{d_{MdR} + \left(\dfrac{\theta_w + K_s \cdot \rho_s + H \cdot \theta_a}{\theta_{w,MdR} + K_{s,MdR} \cdot \rho_{MdR} + H \cdot \theta_{a,MdR}} \right) \left(L_{gw} - L_{MdR} - d_{MdR} \right)} \qquad \text{(optional)}$$

Nomenclature

d_{MdR} = *Thickness of backfill materials (cm)*
L_{gw} = *Depth to groundwater. (cm)*
L_{MdR} = *Depth to backfill materials (cm)*
v_{gw}= *Groundwater Darcy velocity (cm/s)*
K_{sat}= *Hydraulic Conductivity (cm/s)*
I_{eff} = *Infiltration Rate (cm/s)*
τ_{LF} = *Averaging time for leachate flux (s)*
$\theta_{w,MdR}$ = *Volumetric water content in the backfill material (-)*
$\theta_{a,MdR}$ = *Volumetric air content in the backfill material (-)*
$\theta_{e,MdR}$ = *Effective porosity in the backfill material (-)*
H = Henry's law constant (-)
ρ_{MdR} = *Bulk density of backfill material (g/cm^3)*
f_{oc} = *Organic Carbon Fraction (-)*
d_a = *Groundwater Thickckness (cm)*
W = Width of source area parallel to groundwater flow direction (cm)
α_z = *Vertical Dispersivity (cm)*
BDF_{LF} = *Biodegradation factor (-)*

APP. 3C. F&T FACTORS (INT. CHARACTERIZATION)

The fate and transport factors considered in Risk-net for the integrative characterization (i.e. soil-gas, flux chambers and leaching tests) are:

Soil-gas

- α_{samb}: outdoor volatilization factor
- α_{sesp}: indoor volatilization factor

Flux chamber

- α_{FC}: outdoor volatilization factor (open flux chamber)
- $\alpha_{FC(flux)}$: outdoor volatilization factor (open and closed flux chamber)

Eluate

- α_{LFss}: leaching factor from surface soil
- α_{LFsp}: leaching factor from subsurface soil

The main assumptions on which are based the equations are:
- The concentration of pollutants in soil is uniformly distributed and constant throughout the entire exposure period;
- Soil is homogeneous and isotropic and incoherent;
- No biodegradation (with the exception of *DAF*) or other mechanisms of degradation / transformation of pollutants.

Table 60. Soil-gas: Outdoor Volatilization

$$\alpha_{samb}\left[\frac{mg/m^{3}{}_{air}}{mg/m^{3}{}_{soil-gas}}\right]=\frac{BDF_{Vol}}{1+\dfrac{U_{air}\cdot\delta_{air}\cdot L_{sg}}{D_{s}^{eff}\cdot W'}}$$

Nomenclature
L_{sg} = Soil Gas Probe Depth (cm)
D_s^{eff} = Effective diffusivity in the vadose zone (cm^2/s)
W' = Width of source area parallel to wind direction (cm)
δ_{air} = Ambient air mixing zone height (cm)
U_{air} = Wind speed (cm/s)
BDF_{Vol} = Biodegradation factor (-)

Note that in the software it is possible to use empirical attenuation factors instead of the factors calculated with the fate and transport models.

Table 61. Flux Chamber: Outdoor Volatilization

Open flux chamber (Input: Concentration)

$$\alpha_{FC}\left[\frac{mg/m^{3}{}_{air}}{mg/m^{3}{}_{soil-gas}}\right]=\frac{1}{\dfrac{U_{air}\cdot\delta_{air}\cdot A_{fc}}{W'\cdot Q_{in}}}$$

Nomenclature
W' = Width of source area parallel to wind direction (cm)
δ_{air} = Ambient air mixing zone height (cm)
U_{air} = Wind speed (cm/s)
Qin = Flowrate of the carrier gas in the chamber (cm^3/s)
Afc = Chamber surface exposed to soil (cm^2)

Open and closed flux chamber (Input: Flux)

$$\alpha_{FC(flux)}\left[\frac{s}{m}\right]=\frac{1}{\dfrac{U_{air}\cdot\delta_{air}}{W'}}$$

Nomenclature
W' = Width of source area parallel to wind direction (cm)
δ_{air} = Ambient air mixing zone height (cm)
U_{air} = Wind speed (cm/s)

Table 62. Soil-gas: Indoor Volatilization

No differential outdoor/indoor pressure (Δp=0)

$$\alpha_{sesp}\left[\frac{mg/m^3{}_{air}}{mg/m^3{}_{soil-gas}}\right]=\frac{\dfrac{D_s^{eff}}{\left(L_{sg}-Z_{crack}\right)L_b\cdot ER}}{1+\dfrac{D_s^{eff}}{\left(L_{sg}-Z_{crack}\right)L_b\cdot ER}+\dfrac{D_s^{eff}\cdot L_{crack}}{D_{crack}^{eff}\left(L_{sg}-Z_{crack}\right)\eta}}BDF_{Vol}$$

Differential outdoor/indoor pressure (Δp≠0)

$$\alpha_{sesp}\left[\frac{mg/m^3{}_{air}}{mg/m^3{}_{soil-gas}}\right]=\frac{\dfrac{D_s^{eff}}{\left(L_{sg}-Z_{crack}\right)L_b\cdot ER}\cdot e^{\xi}}{e^{\xi}+\dfrac{D_s^{eff}}{\left(L_{sg}-Z_{crack}\right)L_b\cdot ER}+\dfrac{D_s^{eff}\cdot A_b}{Q_s\cdot\left(L_{sg}-Z_{crack}\right)}\cdot(e^{\xi}-1)}BDF_{Vol}$$

Convective Air Flow Through Foundation Cracks, Q_s (cm^3/s)

$$Q_s=\frac{2\pi\cdot\Delta p\cdot k_v\cdot X_{crack}}{\mu_{air}\cdot\ln\left(\dfrac{2\cdot Z_{crack}\cdot X_{crack}}{A_b\cdot\eta}\right)}\qquad\qquad \xi=\frac{Q_s\cdot L_{crack}}{D_{crack}^{eff}\cdot A_b\cdot\eta}$$

Nomenclature

L_{crack} = Thickness foundations (cm)
L_b = Enclosed space volume/infiltration area ratio (cm)
Z_{crack} = Depth to base of enclosed space foundation (cm)
d_s = Thickness of subsurface soil source (cm)
L_{sg} = Soil Gas Probe Depth (cm)
D_s^{eff} = Effective diffusivity in the vadose zone (cm^2/s)
D_{crack}^{eff} = Effective diffusivity in the foundations (cm^2/s)
τ_{indoor} = Averaging time for vapor flux (s)
ER = Enclosed-space air exchange rate (1/s)
η = Areal fraction of cracks in foundations/walls (-)
θ_w = Volumetric water content in the vadose zone (-)
θ_a = Volumetric air content in the vadose zone (-)
θ_e = Effective porosity in the vadose zone (-)
H = Henry's law constant (-)
ρ_s = Soil bulk density (g/cm^3)
X_{crack} = Enclosed space foundation perimeter (cm)
Δp = Differential indoor/outdoor air pressure (g/cm^2/s)
k_v = Soil vapor permeability (cm^2)
A_b = Area of building foundation (cm^2)
μ_{air} = Vapor Viscosity (g/cm/s)
BDF_{Vol} = Biodegradation factor (-)

Note that in the software it is possible to use empirical attenuation factors instead of the factors calculated with the fate and transport models.

Table 63. Flux Chamber: Indoor Volatilization

Open flux chamber (Input: Concentration)

$$\alpha_{FC,indoor}\left[\frac{mg/m^3{}_{air}}{mg/m^3{}_{soil-gas}}\right]=\frac{1}{\frac{L_b\cdot ER\cdot A_{fc}}{Q_{in}}}$$

Nomenclature

L_b = Enclosed space volume/infiltration area ratio (cm)
ER = Enclosed-space air exchange rate (1/s)
Qin = Flowrate of the carrier gas in the chamber (cm^3/s)
Afc = Chamber surface exposed to soil (cm^2)

Open and closed flux chamber (Input: Flux)

$$\alpha_{FC(flux),indoor}\left[\frac{s}{m}\right]=\frac{1}{L_b\cdot ER}$$

Nomenclature

L_b = Enclosed space volume/infiltration area ratio (cm)
ER = Enclosed-space air exchange rate (1/s)

Table 64. Eluate Surface Soil: Leaching to groundwater

$$\alpha_{LFss}\left[\frac{mg/L_{water}}{mg/L_{eluate}}\right]=\frac{SAM}{LDF}BDF_{LF}$$

Soil Attenuation model, SAM (-)

$$SAM=\frac{d}{L_{gw}-L_{s(SS)}}\qquad \text{(optional)}$$

Leachate Dilution Factor, LDF (-)

$$LDF=1+\frac{v_{gw}\cdot\delta_{gw}}{I_{eff}\cdot W}$$

Groundwater mixing zone thickness, *δ_{gw}* *(cm)*

$$\delta_{gw}=(2\cdot 0.0056\cdot W^2)^{0,5}+d_a\cdot\left[1-\exp\left(-\frac{W\cdot I_{eff}}{v_{gw}\cdot d_a}\right)\right]\qquad \text{If } \delta_{gw}>d_a\ \rightarrow\ \delta_{gw}=d_a$$

Nomenclature

L_{gw} = *Depth to groundwater (cm)*
d = Surface Soil Source Thickness (cm)
$L_{s\,(SS)}$ = *Depth to surface soil source (cm)*
v_{gw}= *Groundwater Darcy velocity (cm/s)*
I_{eff} = *Infiltration Rate (cm/s)*
d_a = *Groundwater Thickness (cm)*
W = Width of source area parallel to groundwater flow direction (cm)
α_z = *Vertical Dispersivity (cm)*
BDF_{LF} = *Biodegradation factor (-)*

Table 65. Eluate Subsurface Soil: Leaching to groundwater

$$\alpha_{LFsp}\left[\frac{mg/L_{water}}{mg/L_{eluate}}\right]=\frac{SAM}{LDF}BDF_{LF}$$

Soil Attenuation model, SAM (-)

$$SAM=\frac{d}{L_{gw}-L_{s(SP)}}\qquad \text{(optional)}$$

Leachate Dilution Factor, LDF (-)

$$LDF=1+\frac{v_{gw}\cdot\delta_{gw}}{I_{eff}\cdot W}$$

Groundwater mixing zone thickness, δ_{gw} *(cm)*

$$\delta_{gw}=(2\cdot 0.0056\cdot W^{2})^{0,5}+d_{a}\cdot\left[1-\exp\left(-\frac{W\cdot I_{eff}}{v_{gw}\cdot d_{a}}\right)\right]\qquad \text{If } \delta_{gw}>d_{a}\ \rightarrow\ \delta_{gw}=d_{a}$$

Nomenclature

L_{gw} = Depth to groundwater (cm)
d = Subsurface Soil Source Thickness (cm)
$L_{s\ (SP)}$ = Depth to subsurface soil source (cm)
v_{gw}= Groundwater Darcy velocity (cm/s)
I_{eff} = Infiltration Rate (cm/s)
d_{a} = Groundwater Thickness (cm)
W = Width of source area parallel to groundwater flow direction (cm)
α_{z} = Vertical Dispersivity (cm)
BDF_{LF} = Biodegradation factor (-)

APP. 4. INTAKE RATES

The exposure factors are used to describe the expected behavior for the different receptors within or near the site. Namely these models allow to calculate the average ingested or inhaled dose over the lifetime of the receptor.
The exposure pathways considered in the software are:

- Dermal contact with soil
- Ingestion of soil
- Inhalation of vapors in outdoor environments
- Inhalation of vapors in indoor environments
- Inhalation of particulate matter in outdoor environments
- Inhalation of particulate matter in indoor environments
- Inhalation of particulate matter in outdoor environments
- Inhalation of particulate matter in indoor environments
- Ingestion of water

The types of receptors considered are:

Residential or Recreational Scenario

a) Exposure Mediated (Child and Adult)
b) Exposure Mediated (Child, Teenager, adult and Senior)
c) Child
d) Adult

Commercial or Industrial Scenario

e) Adult Worker

For the residential or recreation exposure scenarios, the software can calculate an average exposure value (options a and b) in order to adjust for varying body weights, exposure durations, skin areas:

$$EM_{adj}(\text{canc.}) = \begin{cases} EM_{child} + EM_{adult} & \text{(option A)} \\ EM_{child} + EM_{teenager} + EM_{adult} + EM_{senior} & \text{(option B)} \end{cases}$$

$$EM_{adj}(\text{non-canc.}) = \begin{cases} EM_{child} & \text{(default)} \\ \max(EM_{child}; EM_{teenager}; EM_{adult}; EM_{senior}) & \text{(if activated)} \end{cases}$$

Similarly, exposure factors calculated using the "reference concentration method" (EC) in the case of average exposure are equal to:

$$EC_{adj}(\text{canc.}) = \begin{cases} EC_{child} + EC_{adult} & \text{(option A)} \\ EC_{child} + EC_{teenager} + EC_{adult} + EC_{senior} & \text{(option B)} \end{cases}$$

$$EC_{adj}(\text{non-canc.}) = \begin{cases} EC_{child} & \text{(default)} \\ \max(EC_{child}; EC_{teenager}; EC_{adult}; EC_{senior}) & \text{(if activated)} \end{cases}$$

The following table reports the equations implemented in the software for the different exposure pathway to calculate the intake rates using the "reference dose" method (EM) and the "reference concentrations" method (EC).

Dermal Contact

$$EM\left[\frac{mg}{kg \times day}\right] = \frac{SA \cdot AF \cdot ABS \cdot EF \cdot ED}{BW \cdot AT \cdot 365 \, \frac{days}{year}}$$

BW = Body weight (kg)
EF = Exposure frequency (d/year)
ED = Exposure Duration (years)
AT = Averaging time (years) (*)
SA = Skin Surface Area (cm^2)
AF = Soil Dermal adherence factor (mg/(cm^2 d)
ABS = Dermal adsorption factor (-)

Soil ingestion

$$EM\left[\frac{mg}{kg \times day}\right] = \frac{IR \cdot FI \cdot EF \cdot ED}{BW \cdot AT \cdot 365 \, \frac{days}{year}}$$

BW = Body weight (kg)
EF = Exposure frequency (d/year)
ED = Exposure Duration (years)
AT = Averaging time (years) (*)
IR = Soil Ingestion rate (mg/ d)
FI = Soil ingestion fraction (-)

Outdoor Vapors and Dust Inhalation

$$EM\left[\frac{m^3}{kg \times day}\right] = \frac{B_o \cdot EF_{go} \cdot EF \cdot ED}{BW \cdot AT \cdot 365 \, \frac{days}{year}}$$

BW = Body weight (kg)
EF = Exposure frequency (d/year)
ED = Exposure Duration (years)
AT = Averaging time (years) (*)
EF_{go} = Daily Outdoor Exposure frequency (h/d)
B_o = Outdoor Inhalation rate (m^3/h)

Indoor Vapors and Dust Inhalation

$$EM\left[\frac{m^3}{kg \times day}\right] = \frac{B_i \cdot EF_{gi} \cdot EF \cdot ED}{BW \cdot AT \cdot 365 \, \frac{days}{year}}$$

BW = Body weight (kg)
EF = Exposure frequency (d/year)
ED = Exposure Duration (years)
AT = Averaging time (years) (*)
EF_{gi} = Daily Indoor Exposure frequency (h/d)
B_i = Indoor Inhalation rate (m^3/h)

Water Ingestion

$$EM\left[\frac{L}{kg \times day}\right] = \frac{IR_w \cdot EF \cdot ED}{BW \cdot AT \cdot 365 \, \frac{days}{year}}$$

BW = Body weight (kg)
EF = Exposure frequency (d/year)
ED = Exposure Duration (years)
AT = Averaging time (years) (*)
IR_w = Water Ingestion rate (L/d)

(*) For non-carcinogenic contaminants AT = ED

APP. 5. USING ADVANCED CHARACTERIZATION DATA

By default, in the software the data obtained in the advanced characterization of the site (soil-gas, flux-chamber, air measurements and leaching tests) are exclusively used to calculate the risks for the receptors. However, the user from the model options screen ("Advanced Characterization" screen) can decide whether to use these data also for the modulation of SSTLs in the different environmental media (surface soil, subsurface soil and groundwater). In this case, the data obtained from these monitoring campaigns are used to calculate semi-empirical transport factors for the selected sources that are used to calculate the new SSTLs.

The calculation of the empirical and semi-empirical transport factors are described in the following sections.

Outdoor air measurements

Outdoor air measurements can be used to estimate the site-specific attenuation of vapors observed in the field. In particular, by measuring the concentration in the air and the concentration in the source (soil or groundwater) it is possible to estimate the attenuation of the contaminants during transport from the source at the point of exposure.

This factor, defined with the symbol β, can be estimated in the case of soil or groundwater using the following equations:

<u>Volatilization from soil</u>

$$\beta_{soil(AR,Outdoor)}\left[\frac{mg/m^3}{mg/kg}\right]=\frac{C_{air,outdoor}}{C_{soil}}$$

<u>Volatilization from groundwater</u>

$$\beta_{gw(AR,Outdoor)}\left[\frac{mg/m^3}{mg/L}\right]=\frac{C_{air,outdoor}}{C_{groundwater}}$$

where:

$C_{air,outdoor}$ = *Ambient Air Concentration (mg/m^3)*
C_{soil} = *Concentration in the soil (mg/kg)*
$C_{groundwater}$ = *Concentration in groundwater (mg/L)*

The β values can be calculated automatically by the software based on the concentrations defined in the source and in the outdoor air.

Once the site-specific β factors have been estimated from the experimental data obtained from the monitoring campaigns, it is therefore possible to estimate the site-specific transport factors as described below.

Outdoor Volatilization

$$VF_{samb,empirical}\left[\frac{mg/m^3}{mg/kg}\right]=\beta_{soil(AR,Outdoor)}$$

$$VF_{wamb,empirical}\left[\frac{mg/m^3}{mg/L}\right]=\beta_{gw(AR,Outdoor)}$$

The above site-specific fate and transport factors are then used in the standard equations described in the previous section for the calculation of the new SSTLs.

Indoor air measurements

Indoor air measurements can be used to estimate the site-specific attenuation of vapors observed in the field. In particular, by measuring the concentration in the building and the concentration in the source (soil or groundwater) it is possible to estimate the attenuation of the contaminants during transport from the source at the point of exposure.
This factor, defined with the symbol β, can be estimated in the case of soil or groundwater using the following equations:

Volatilization from soil

$$\beta_{soil(AR,Indoor)}\left[\frac{mg/m^3}{mg/kg}\right]=\frac{C_{air,indoor}}{C_{soil}}$$

Volatilization from groundwater

$$\beta_{gw(AR,Indoor)}\left[\frac{mg/m^3}{mg/L}\right]=\frac{C_{air,indoor}}{C_{groundwater}}$$

where:
$C_{air,indoor}$ = *Indoor Air Concentration (mg/m^3)*
C_{soil} = *Concentration in the soil (mg/kg)*
$C_{groundwater}$ = *Concentration in groundwater (mg/L)*

The β values can be calculated automatically by the software based on the concentrations defined in the source and in the indoor air.
Once the site-specific β factors have been estimated from the experimental data obtained from the monitoring campaigns, it is therefore possible to estimate the site-specific transport factors as described below.

Indoor Volatilization

$$VF_{sesp,empirical}\left[\frac{mg/m^3}{mg/kg}\right]=\beta_{soil(AR,Indoor)}$$

$$VF_{wesp,empirical}\left[\frac{mg/m^3}{mg/L}\right]=\beta_{gw(AR,Indoor)}$$

The above site-specific fate and transport factors are then used in the standard equations described in the previous section for the calculation of the new SSTLs.

Soil-gas measurements

Soil-gas measurements can be used to assess the site-specific attenuation of vapors observed in the field. In particular, by measuring the concentration in the soil-gas and the concentration in the source (soil or groundwater) it is possible to estimate the attenuation of the contaminants during transport from the source at the soil-gas probe depth.
This factor, defined with the symbol β, can be estimated in the case of soil or groundwater using the following equations:

Volatilization from soil

$$\beta_{soil(SG)}\left[\frac{mg/m^3}{mg/kg}\right]=\frac{C_{soil-gas}}{C_{soil}}$$

Volatilization from groundwater

$$\beta_{fgw(SG)}\left[\frac{mg/m^3}{mg/L}\right]=\frac{C_{soil-gas}}{C_{groundwater}}$$

where:
$C_{soil\text{-}gas}$ = *Soil-gas Concentration (mg/m^3)*
C_{soil} = *Concentration in the soil (mg/kg)*
$C_{groundwater}$ = *Concentration in groundwater (mg/L)*

The β values can be calculated automatically by the software based on the concentrations defined in the source and in the soil gas.
Once the site-specific β factors have been estimated from the experimental data obtained from the monitoring campaigns, it is therefore possible to estimate the site-specific transport factors as described below.

Outdoor Volatilization

$$VF_{samb,semi-empirical}\left[\frac{mg/m^3}{mg/kg}\right]=\beta_{soil(SG)}\cdot\alpha_{samb}$$

$$VF_{wamb,semi-empirical}\left[\frac{mg/m^3}{mg/L}\right]=\beta_{gw(SG)}\cdot\alpha_{samb}$$

Indoor Volatilization

$$VF_{sesp,semi-empirical}\left[\frac{mg/m^3}{mg/kg}\right]=\beta_{soil(SG)}\cdot\alpha_{sesp}$$

$$VF_{wesp,semi-empirical}\left[\frac{mg/m^3}{mg/L}\right]=\beta_{gw(SG)}\cdot\alpha_{sesp}$$

The above site-specific fate and transport factors are then used in the standard equations described in the previous section for the calculation of the new SSTLs.

Flux Chambers measurements

Flux-chambers data can be used to assess the site-specific attenuation of vapors observed in the field. In particular, by measuring the concentration in the flux chamber and the concentration in the source (soil or groundwater), it is possible to estimate the attenuation of the contaminants during transport from the source to the ground surface. This factor, defined with the symbol β, can be estimated in the case of soil or groundwater using the following equations:

Volatilization from soil (open chambers)

$$\beta_{soil(FC)}\left[\frac{mg/m^3}{mg/kg}\right]=\frac{C_{FC}}{C_{soil}}$$

Volatilization from groundwater (open chambers)

$$\beta_{gw(FC)}\left[\frac{mg/m^3}{mg/L}\right]=\frac{C_{FC}}{C_{groundwater}}$$

where:
C_{FC} = Concentration in the flux chamber (mg/m^3)
C_{soil} = Concentration in the soil (mg/kg)
$C_{groundwater}$ = Concentration in groundwater (mg/L)

Volatilization from soil (open and closed chambers)

$$\beta_{soil(FC-flux)}\left[\frac{mg/m^2/s}{mg/kg}\right]=\frac{F}{C_{soil}}$$

Volatilization from groundwater (open and closed chambers)

$$\beta_{gw(FC-flux)}\left[\frac{mg/m^2/s}{mg/L}\right]=\frac{F}{C_{groundwater}}$$

where:

F = Measured flux (mg/m²/s)
C_{soil} *= Concentration in the soil (mg/kg)*
$C_{groundwater}$ *= Concentration in groundwater (mg/L)*

The β values can be calculated automatically by the software based on the concentrations defined in the source and in the flux chambers.
Once the site-specific β factors have been estimated from the experimental data obtained from the monitoring campaigns, it is therefore possible to estimate the site-specific transport factors as described below.

Outdoor Volatilization (open chambers)

$$VF_{samb,semi-empirical}\left[\frac{mg/m^3}{mg/kg}\right]=\beta_{soil(FC)}\cdot\alpha_{FC}$$
$$VF_{wamb,semi-empirical}\left[\frac{mg/m^3}{mg/L}\right]=\beta_{fgw(FC)}\cdot\alpha_{FC}$$

Outdoor Volatilization (open and closed chambers)

$$VF_{samb,semi-empirical}\left[\frac{mg/m^3}{mg/kg}\right]=\beta_{soil(FC-flux)}\cdot\alpha_{FC(flux)}$$
$$VF_{wamb,semi-empirical}\left[\frac{mg/m^3}{mg/L}\right]=\beta_{gw(FC-flux)}\cdot\alpha_{FC(flux)}$$

The above site-specific fate and transport factors are then used in the standard equations described in the previous section for the calculation of the new SSTLs.

Leaching Tests

I risultati del test di cessione possono essere utilizzati per valutare la ripartizione sito-specifica dei vapori osservata sul campo. In particolare, misurando la concentrazione nell'eluato e la concentrazione in sorgente (localizzata nel terreno o nelle acque sotterranee) è possibile la ripartizione tra il contaminante in sorgente e in fase disciolta nell'acqua interstiziale.
The results of the leaching tests can be used to evaluate the site-specific partition of the contaminants observed in the field. In particular, by measuring the concentration in the eluate and the concentration in the source (soil or groundwater) it is possible to estimate the partition between the contaminant in the source and in the dissolved phase in the interstitial water.
This factor, defined with the symbol β, can be estimated in the case of soil or groundwater using the following equations:

Eluate – Surface Soil

$$\beta_{ss(LF)}\left[\frac{mg/L}{mg/kg}\right]=\frac{C_{eluate,ss}}{C_{ss}}$$

Eluate – Subsurface Soil

$$\beta_{sp(LF)}\left[\frac{mg/L}{mg/kg}\right]=\frac{C_{eluato,sp}}{C_{sp}}$$

where:
$C_{eluato,ss}$ *= Concentration in the eluate of the leaching test carried out on the surface soil (mg/L)*
C_{ss} *= Concentration in surface soil (mg/kg)*
$C_{eluato,sp}$ *= Concentration in the eluate of the leaching test carried out on the subsurface soil (mg/L)*
C_{sp} *= Concentration in subsurface soil (mg/kg)*

The β values can be calculated automatically by the software based on the concentrations defined in the source and in the eluates.
Once the site-specific β factors have been estimated from the experimental data obtained from the monitoring campaigns, it is therefore possible to estimate the site-specific transport factors as described below.

Leaching from surface soil

$$LF_{ss,semi-empirical}\left[\frac{mg/L}{mg/kg}\right]=\beta_{ss(LF)}\cdot\alpha_{LFss}$$

Leaching from subsurface soil

$$LF_{sp,semi-empirical}\left[\frac{mg/L}{mg/kg}\right]=\beta_{sp(LF)}\cdot\alpha_{LFsp}$$

The above site-specific fate and transport factors are then used in the standard equations described in the previous section for the calculation of the new SSTLs.

APP. 6. DETAILED CONCENTRATIONS

On the "Concentration Detail" screen the user can check the expected concentrations in the soil-gas, eluate, outdoor air, indoor air based on the total concentrations defined by the user in the source (Surface Soil, Subsurface Soil or Groundwater). This appendix shows the equations used by the software for these estimates.

Table 66. Concentrations expected in air

Outdoor Volatilization

From Surface Soil

$$C_{Air.Outdoor(ss)} = C_{ss} \cdot VF_{ss}$$

From Subsurface Soil

$$C_{Air.Outdoor(sp)} = C_{sp} \cdot VF_{samb}$$

From Groundwater

$$C_{Air.Outdoor(gw)} = C_{gw} \cdot VF_{wamb}$$

Indoor Volatilization

From Surface Soil

$$C_{Air.Indoor(ss)} = C_{ss} \cdot VF_{ssesp}$$

From Subsurface Soil

$$C_{Air.Indoor(sp)} = C_{sp} \cdot VF_{sesp}$$

From Groundwater

$$C_{Air.Indoor(gw)} = C_{gw} \cdot VF_{wesp}$$

Nomenclature

$C_{Air.Outdoor}$: *concentration expected in outdoor air (mg/m^3)*
$C_{Air.Indoor}$: *concentration expected in indoor air (mg/m^3)*
C_{ss}: *concentration measured in the surface soil (mg/kg)*
C_{sp}: *concentration measured in the subsurface soil (mg/kg)*
C_{gw}: *concentration measured in groundwater (mg/L)*

For the meaning of the other symbols, readers are directed to the previous appendices.

Table 67. Concentrations expected in soil gas (outdoor)

Outdoor Volatilization

From Surface Soil

$$C_{sg.Outdoor(ss)} = C_{ss} \cdot \frac{VF_{ss}}{\alpha_{samb}}$$

$$C_{sg(ss)} = C_{ss} \cdot K_{ws} \cdot H \cdot 1000$$ *(if selected by the user)*

From Subsurface Soil

$$C_{sg.Outdoor(sp)} = C_{sp} \cdot \frac{VF_{samb}}{\alpha_{samb}}$$

$$C_{sg(sp)} = C_{sp} \cdot K_{ws} \cdot H \cdot 1000$$ *(if selected by the user)*

From Groundwater

$$C_{sg.Outdoor(gw)} = C_{gw} \cdot \frac{VF_{wamb}}{\alpha_{samb}}$$

$$C_{sg(gw)} = C_{gw} \cdot K_{ws} \cdot H \cdot 1000$$ *(if selected by the user)*

Nomenclature

$C_{sg.Outdoor}$: *concentration expected in the soil gas for the outdoor volatilization pathway (mg/m^3)*
C_{ss}: *concentration measured in the surface soil (mg/kg)*
C_{sp}: *concentration measured in the subsurface soil (mg/kg)*
C_{gw}: *concentration measured in groundwater (mg/L)*

For the meaning of the other symbols, readers are directed to the previous appendices.

Table 68. Concentrations expected in soil gas (indoor)

Indoor Volatilization

From Surface Soil

$$C_{sg.Indoor(ss)} = C_{ss} \cdot \frac{VF_{ssesp}}{\alpha_{sesp}}$$

$$C_{sg(ss)} = C_{ss} \cdot K_{ws} \cdot H \cdot 1000$$ *(if selected by the user)*

From Subsurface Soil

$$C_{sg.Indoor(sp)} = C_{sp} \cdot \frac{VF_{sesp}}{\alpha_{sesp}}$$

$$C_{sg(sp)} = C_{sp} \cdot K_{ws} \cdot H \cdot 1000$$ *(if selected by the user)*

From Groundwater

$$C_{sg.Indoor(gw)} = C_{gw} \cdot \frac{VF_{wesp}}{\alpha_{sesp}}$$

$$C_{sg(gw)} = C_{gw} \cdot K_{ws} \cdot H \cdot 1000$$ *(if selected by the user)*

Nomenclature

$C_{sg.Indoor}$: *concentration expected in the soil gas for the indoor volatilization pathway (mg/m^3)*

C_{ss}: *concentration measured in the surface soil (mg/kg)*

C_{sp}: *concentration measured in the subsurface soil (mg/kg)*

C_{gw}: *concentration measured in groundwater (mg/L)*

For the meaning of the other symbols, readers are directed to the previous appendices.

Table 69. Concentrations expected in the flux chamber

Outdoor Volatilization

From Surface Soil

$$C_{FC(ss)} = C_{ss} \cdot \frac{K_{ws} \cdot H \cdot 1000}{\alpha_{FC}}$$

From Subsurface Soil

$$C_{FC(sp)} = C_{sp} \cdot \frac{VF_{samb}(1)}{\alpha_{FC}}$$

From Groundwater

$$C_{FC(gw)} = C_{gw} \cdot \frac{VF_{wamb}}{\alpha_{FC}}$$

Nomenclature

C_{fc}: concentration expected in the flux chamber (mg/m^3)
C_{ss}: concentration measured in the surface soil (mg/kg)
C_{sp}: concentration measured in the subsurface soil (mg/kg)
C_{gw}: concentration measured in groundwater (mg/L)

For the meaning of the other symbols, readers are directed to the previous appendices.

Table 70. Concentration expected in the eluate

Leaching from the soil to groundwater

From Surface Soil

$$C_{El(ss)} = C_{ss} \cdot K_{ws(ss)}$$

From Subsurface Soil

$$C_{El(sp)} = C_{sp} \cdot K_{ws(sp)}$$

Nomenclature

C_{El}: concentration expected in the the eluate (mg/L)
C_{ss}: concentration measured in the surface soil (mg/kg)
C_{sp}: concentration measured in the subsurface soil (mg/kg)

For the meaning of the other symbols, readers are directed to the previous appendices.

Table 71. Concentration expected in groundwater

Leaching from the soil to groundwater (POC = 0)

From Surface Soil

$$C_{gw(ss)} = C_{ss} \cdot LF_{ss}$$

From Subsurface Soil

$$C_{gw(sp)} = C_{sp} \cdot LF_{sp}$$

Leaching from the soil to groundwater (POC > 0)

From Surface Soil

$$C_{gw(ss)} = C_{ss} \cdot \frac{LF_{ss}}{DAF}$$

From Subsurface Soil

$$C_{gw(sp)} = C_{sp} \cdot \frac{LF_{sp}}{DAF}$$

Nomenclature

C_{gw}: *concentration expected in groundwater (mg/L)*
C_{ss}: *concentration measured in the surface soil (mg/kg)*
C_{sp}: *concentration measured in the subsurface soil (mg/kg)*

For the meaning of the other symbols, readers are directed to the previous appendices.

APP. 7. AGE DEPENDENT ADJUSTMENT FACTOR (ADAF)

For carcinogenic substances that act through a genotoxic action, the software allows to use an adjustment factor "ADAF" (Age Dependent Adjustment Factor) to be applied to the carcinogenic toxicological parameters (SF Ing., SF Inal., IUR) according to the age of the potentially exposed receptor:

$$SF_{child} = SF \cdot ADAF_{child}$$
$$IUR_{child} = IUR \cdot ADAF_{child}$$

$$SF_{teenager} = SF \cdot ADAF_{teenager}$$
$$IUR_{teenager} = IUR \cdot ADAF_{teenager}$$

In the default database of the software are defined for Benzo(a)pyrene, Dibenzo(a,h)anthracene, 1,2,3-Trichloropropane, Dichloromethane, Trichloroethylene and Acrylamide an ADAF factor equal to 5 for the child and 3 for the teenager. For Vinyl Chloride, the ADAF factor for the child in the database is set equal to 2.

APP. 8. KOC AND KD FUNCTION OF PH

For the substances in which the Koc and the Kd are a function of the pH, if the Default Database is used, the values of the distribution coefficients reported in the following tables are adopted in the software according to the pH defined in the site.

Table 72. Koc values as a function of pH for some organic compounds (1/2).

Koc (L/kg) as a function of pH					
pH	**Benzoic Acid**	**2-Chlorophenol**	**Dichlorophenol (2,4)**	**Dinitrophenol (2,4)**	**Pentachlorophenol**
4.9	5.5E+00	3.98E+02	1.59E+02	2.94E-02	9.05E+03
5	4.6E+00	3.98E+02	1.59E+02	2.55E-02	7.96E+03
5.1	3.9E+00	3.98E+02	1.59E+02	2.23E-02	6.93E+03
5.2	3.3E+00	3.98E+02	1.59E+02	1.98E-02	5.97E+03
5.3	2.7E+00	3.98E+02	1.59E+02	1.78E-02	5.10E+03
5.4	2.3E+00	3.98E+02	1.58E+02	1.62E-02	4.32E+03
5.5	1.9E+00	3.97E+02	1.58E+02	1.50E-02	3.65E+03
5.6	1.7E+00	3.97E+02	1.58E+02	1.40E-02	3.07E+03
5.7	1.4E+00	3.97E+02	1.58E+02	1.32E-02	2.58E+03
5.8	1.2E+00	3.97E+02	1.58E+02	1.25E-02	2.18E+03
5.9	1.1E+00	3.97E+02	1.57E+02	1.20E-02	1.84E+03
6	9.7E-01	3.96E+02	1.57E+02	1.16E-02	1.56E+03
6.1	8.8E-01	3.96E+02	1.57E+02	1.13E-02	1.33E+03
6.2	8.0E-01	3.96E+02	1.56E+02	1.10E-02	1.15E+03
6.3	7.4E-01	3.95E+02	1.55E+02	1.08E-02	9.98E+02
6.4	6.9E-01	3.94E+02	1.54E+02	1.06E-02	8.77E+02
6.5	6.5E-01	3.93E+02	1.53E+02	1.05E-02	7.81E+02
6.6	6.2E-01	3.92E+02	1.52E+02	1.04E-02	7.03E+02
6.7	6.0E-01	3.90E+02	1.50E+02	1.03E-02	6.40E+02
6.8	5.8E-01	3.88E+02	1.47E+02	1.02E-02	5.92E+02
6.9	5.6E-01	3.86E+02	1.45E+02	1.02E-02	5.52E+02
7	5.5E-01	3.83E+02	1.41E+02	1.02E-02	5.21E+02
7.1	5.4E-01	3.79E+02	1.38E+02	1.02E-02	4.96E+02
7.2	5.3E-01	3.75E+02	1.33E+02	1.01E-02	4.76E+02
7.3	5.3E-01	3.69E+02	1.28E+02	1.01E-02	4.61E+02
7.4	5.2E-01	3.62E+02	1.21E+02	1.01E-02	4.47E+02
7.5	5.2E-01	3.54E+02	1.14E+02	1.01E-02	4.37E+02
7.6	5.1E-01	3.44E+02	1.07E+02	1.01E-02	4.29E+02
7.7	5.1E-01	3.33E+02	9.84E+01	1.00E-02	4.23E+02
7.8	5.1E-01	3.19E+02	8.97E+01	1.00E-02	4.18E+02
7.9	5.1E-01	3.04E+02	8.07E+01	1.00E-02	4.14E+02
8	5.1E-01	2.86E+02	7.17E+01	1.00E-02	4.10E+02

Table 73. Koc values as a function of pH for some organic compounds (2/2).

Koc (L/kg) as a function of pH

pH	Tetrachlorophenol 2,3,4,5	Tetrachlorophenol 2,4,6	Trichlorophenol 2,4,5	Trichlorophenol 2,4,6
4.9	1.73E+04	4.45E+03	2.37E+03	1.04E+03
5	1.72E+04	4.15E+03	2.36E+03	1.03E+03
5.1	1.70E+04	3.83E+03	2.36E+03	1.02E+03
5.2	1.67E+04	3.49E+03	2.35E+03	1.01E+03
5.3	1.65E+04	3.14E+03	2.34E+03	9.99E+02
5.4	1.61E+04	2.79E+03	2.33E+03	9.82E+02
5.5	1.57E+04	2.45E+03	2.32E+03	9.62E+02
5.6	1.52E+04	2.13E+03	2.31E+03	9.38E+02
5.7	1.47E+04	1.83E+03	2.29E+03	9.10E+02
5.8	1.40E+04	1.56E+03	2.27E+03	8.77E+02
5.9	1.32E+04	1.32E+03	2.24E+03	8.39E+02
6	1.24E+04	1.11E+03	2.21E+03	7.96E+02
6.1	1.15E+04	9.27E+02	2.17E+03	7.48E+02
6.2	1.05E+04	7.75E+02	2.12E+03	6.97E+02
6.3	9.51E+03	6.47E+02	2.06E+03	6.44E+02
6.4	8.48E+03	5.42E+02	1.99E+03	5.89E+02
6.5	7.47E+03	4.55E+02	1.91E+03	5.33E+02
6.6	6.49E+03	3.84E+02	1.82E+03	4.80E+02
6.7	5.58E+03	3.27E+02	1.71E+03	4.29E+02
6.8	4.74E+03	2.80E+02	1.60E+03	3.81E+02
6.9	3.99E+03	2.42E+02	1.47E+03	3.38E+02
7	3.33E+03	2.13E+02	1.34E+03	3.00E+02
7.1	2.76E+03	1.88E+02	1.21E+03	2.67E+02
7.2	2.28E+03	1.69E+02	1.07E+03	2.39E+02
7.3	1.87E+03	1.53E+02	9.43E+02	2.15E+02
7.4	1.53E+03	1.41E+02	8.19E+02	1.95E+02
7.5	1.25E+03	1.31E+02	7.03E+02	1.78E+02
7.6	1.02E+03	1.23E+02	5.99E+02	1.64E+02
7.7	8.31E+02	1.17E+02	5.07E+02	1.53E+02
7.8	6.79E+02	1.13E+02	4.26E+02	1.44E+02
7.9	5.56E+02	1.08E+02	3.57E+02	1.37E+02
8	4.58E+02	1.05E+02	2.98E+02	1.31E+02

Table 74. Kd values as a function of pH for some inorganic contaminants (1/2).

Kd (L/kg) as a function of pH						
pH	**Arsenic**	**Barium**	**Beryllium**	**Cadmium**	**Chromium III**	**Chromium VI**
4.9	2.5E+01	1.1E+01	2.3E+01	1.5E+01	1.2E+03	3.1E+01
5	2.5E+01	1.2E+01	2.6E+01	1.7E+01	1.9E+03	3.1E+01
5.1	2.5E+01	1.4E+01	2.8E+01	1.9E+01	3.0E+03	3.0E+01
5.2	2.6E+01	1.5E+01	3.1E+01	2.1E+01	4.9E+03	2.9E+01
5.3	2.6E+01	1.7E+01	3.5E+01	2.3E+01	8.1E+03	2.8E+01
5.4	2.6E+01	1.9E+01	3.8E+01	2.5E+01	1.3E+04	2.7E+01
5.5	2.6E+01	2.1E+01	4.2E+01	2.7E+01	2.1E+04	2.7E+01
5.6	2.6E+01	2.2E+01	4.7E+01	2.9E+01	3.5E+04	2.6E+01
5.7	2.7E+01	2.4E+01	5.3E+01	3.1E+01	5.5E+04	2.5E+01
5.8	2.7E+01	2.6E+01	6.0E+01	3.3E+01	8.7E+04	2.5E+01
5.9	2.7E+01	2.8E+01	6.9E+01	3.5E+01	1.3E+05	2.4E+01
6	2.7E+01	3.0E+01	8.2E+01	3.7E+01	2.0E+05	2.3E+01
6.1	2.7E+01	3.1E+01	9.9E+01	4.0E+01	3.0E+05	2.3E+01
6.2	2.8E+01	3.3E+01	1.2E+02	4.2E+01	4.2E+05	2.2E+01
6.3	2.8E+01	3.5E+01	1.6E+02	4.4E+01	5.8E+05	2.2E+01
6.4	2.8E+01	3.6E+01	2.1E+02	4.8E+01	7.7E+05	2.1E+01
6.5	2.8E+01	3.7E+01	2.8E+02	5.2E+01	9.9E+05	2.0E+01
6.6	2.8E+01	3.9E+01	3.9E+02	5.7E+01	1.2E+06	2.0E+01
6.7	2.9E+01	4.0E+01	5.5E+02	6.4E+01	1.5E+06	1.9E+01
6.8	2.9E+01	4.1E+01	7.9E+02	7.5E+01	1.8E+06	1.9E+01
6.9	2.9E+01	4.2E+01	1.1E+03	9.1E+01	2.1E+06	1.8E+01
7	2.9E+01	4.2E+01	1.7E+03	1.1E+02	2.5E+06	1.8E+01
7.1	2.9E+01	4.3E+01	2.5E+03	1.5E+02	2.8E+06	1.7E+01
7.2	3.0E+01	4.4E+01	3.8E+03	2.0E+02	3.1E+06	1.7E+01
7.3	3.0E+01	4.4E+01	5.7E+03	2.8E+02	3.4E+06	1.6E+01
7.4	3.0E+01	4.5E+01	8.6E+03	4.0E+02	3.7E+06	1.6E+01
7.5	3.0E+01	4.6E+01	1.3E+04	5.9E+02	3.9E+06	1.6E+01
7.6	3.1E+01	4.6E+01	2.0E+04	8.7E+02	4.1E+06	1.5E+01
7.7	3.1E+01	4.7E+01	3.0E+04	1.3E+03	4.2E+06	1.5E+01
7.8	3.1E+01	4.9E+01	4.6E+04	1.9E+03	4.3E+06	1.4E+01
7.9	3.1E+01	5.0E+01	6.9E+04	2.9E+03	4.3E+06	1.4E+01
8	3.1E+01	5.2E+01	1.0E+05	4.3E+03	4.3E+06	1.4E+01

Table 75. Kd values as a function of pH for some inorganic contaminants (2/2).

Kd (L/kg) as a function of pH

pH	Mercury	Nickel	Silver	Selenium	Thallium	Zinc
4.9	4.0E-02	1.6E+01	1.0E-01	1.8E+01	4.4E+01	1.6E+01
5	6.0E-02	1.8E+01	1.3E-01	1.7E+01	4.5E+01	1.8E+01
5.1	9.0E-02	2.0E+01	1.6E-01	1.6E+01	4.6E+01	1.9E+01
5.2	1.4E-01	2.2E+01	2.1E-01	1.5E+01	4.7E+01	2.1E+01
5.3	2.0E-01	2.4E+01	2.6E-01	1.4E+01	4.8E+01	2.3E+01
5.4	3.0E-01	2.6E+01	3.3E-01	1.3E+01	5.0E+01	2.5E+01
5.5	4.6E-01	2.8E+01	4.2E-01	1.2E+01	5.1E+01	2.6E+01
5.6	6.9E-01	3.0E+01	5.3E-01	1.1E+01	5.2E+01	2.8E+01
5.7	1.0E+00	3.2E+01	6.7E-01	1.1E+01	5.4E+01	3.0E+01
5.8	1.6E+00	3.4E+01	8.4E-01	9.8E+00	5.5E+01	3.2E+01
5.9	2.3E+00	3.6E+01	1.1E+00	9.2E+00	5.6E+01	3.4E+01
6	3.5E+00	3.8E+01	1.3E+00	8.6E+00	5.8E+01	3.6E+01
6.1	5.1E+00	4.0E+01	1.7E+00	8.0E+00	5.9E+01	3.9E+01
6.2	7.5E+00	4.2E+01	2.1E+00	7.5E+00	6.1E+01	4.2E+01
6.3	1.1E+01	4.5E+01	2.7E+00	7.0E+00	6.2E+01	4.4E+01
6.4	1.6E+01	4.7E+01	3.4E+00	6.5E+00	6.4E+01	4.7E+01
6.5	2.2E+01	5.0E+01	4.2E+00	6.1E+00	6.6E+01	5.1E+01
6.6	3.0E+01	5.4E+01	5.3E+00	5.7E+00	6.7E+01	5.4E+01
6.7	4.0E+01	5.8E+01	6.6E+00	5.3E+00	6.9E+01	5.8E+01
6.8	5.2E+01	6.5E+01	8.3E+00	5.0E+00	7.1E+01	6.2E+01
6.9	6.6E+01	7.4E+01	1.0E+01	4.7E+00	7.3E+01	6.8E+01
7	8.2E+01	8.8E+01	1.3E+01	4.3E+00	7.4E+01	7.5E+01
7.1	9.9E+01	1.1E+02	1.6E+01	4.1E+00	7.6E+01	8.3E+01
7.2	1.2E+02	1.4E+02	2.0E+01	3.8E+00	7.8E+01	9.5E+01
7.3	1.3E+02	1.8E+02	2.5E+01	3.5E+00	8.0E+01	1.1E+02
7.4	1.5E+02	2.5E+02	3.1E+01	3.3E+00	8.2E+01	1.3E+02
7.5	1.6E+02	3.5E+02	3.9E+01	3.1E+00	8.5E+01	1.6E+02
7.6	1.7E+02	4.9E+02	4.8E+01	2.9E+00	8.7E+01	1.9E+02
7.7	1.8E+02	7.0E+02	5.9E+01	2.7E+00	8.9E+01	2.4E+02
7.8	1.9E+02	9.9E+02	7.3E+01	2.5E+00	9.1E+01	3.1E+02
7.9	1.9E+02	1.4E+03	8.9E+01	2.4E+00	9.4E+01	4.0E+02
8	2.0E+02	1.9E+03	1.1E+02	2.2E+00	9.6E+01	5.3E+02