

RISK-NET



USER GUIDE

Version 3.3
May 2026

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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Acknowledgments

The authors would like to thank the researchers, consulting professionals, and regulatory agency staff who, throughout the development and evolution of the software, contributed valuable feedback, reports, and suggestions that helped improve the functionality of Risk-net.

Ref: Verginelli I. (2026). Risk-net User Guide. Version 3.3. Rome, Italy, Reconnet.

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

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DESCRIPTION OF THE SOFTWARE

The Risk-net software has been developed by the University of Rome Tor Vergata 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 levels 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.

INTERFACE AND SOFTWARE USE

Program Installation. Risk-net is developed using JavaScript and HTML technologies. Version 3.3 is distributed as a Progressive Web App (PWA). The application can therefore be used directly through a web browser or installed locally on a device (using the “Install App” button). Installing the PWA does not require administrator privileges on the device. Unlike previous versions, Risk-net 3.3 is compatible with major desktop platforms (Windows, macOS, Linux) as well as mobile platforms (iOS, Android). As a result, the application can be used on computers, tablets, and smartphones while maintaining the same core functionality.

Program Launch. To start the program, simply open the “Risk-net” application (or use the shortcut available on the desktop or in the applications menu/taskbar).

Software Activation. Upon first launch, users must review and accept the terms of use in order to proceed, by selecting the appropriate confirmation checkbox. Use of the software is subject to acceptance of these terms. By accessing and using the application, the user implicitly declares that they have read and fully accepted the terms and conditions.

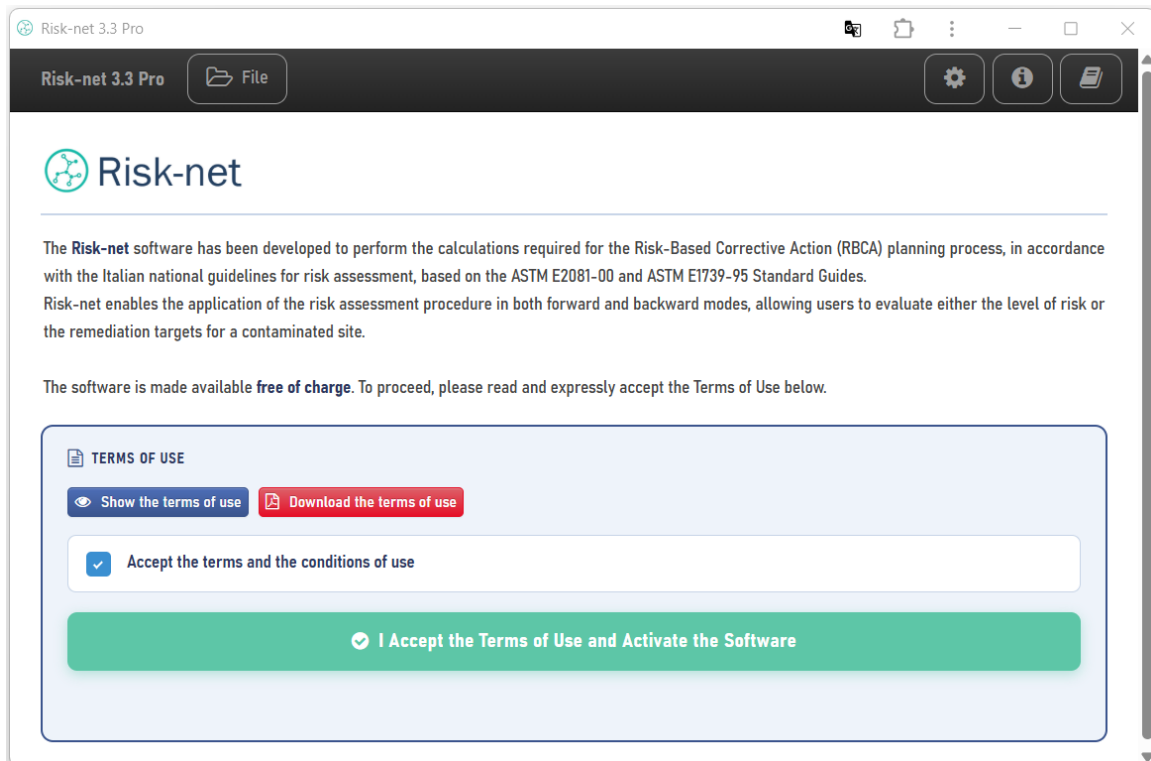


Figure 1. Risk-net activation.

Optimal Screen Resolution. The optimal display of Risk-net is achieved with a screen resolution of at least 1024 × 768 pixels.

The software can still be used on devices with smaller screens; however, in such cases some interface elements may require scrolling or zoom adjustments for proper viewing.

MAIN SCREEN

The main screen is automatically opened at startup (Figure 2). 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.

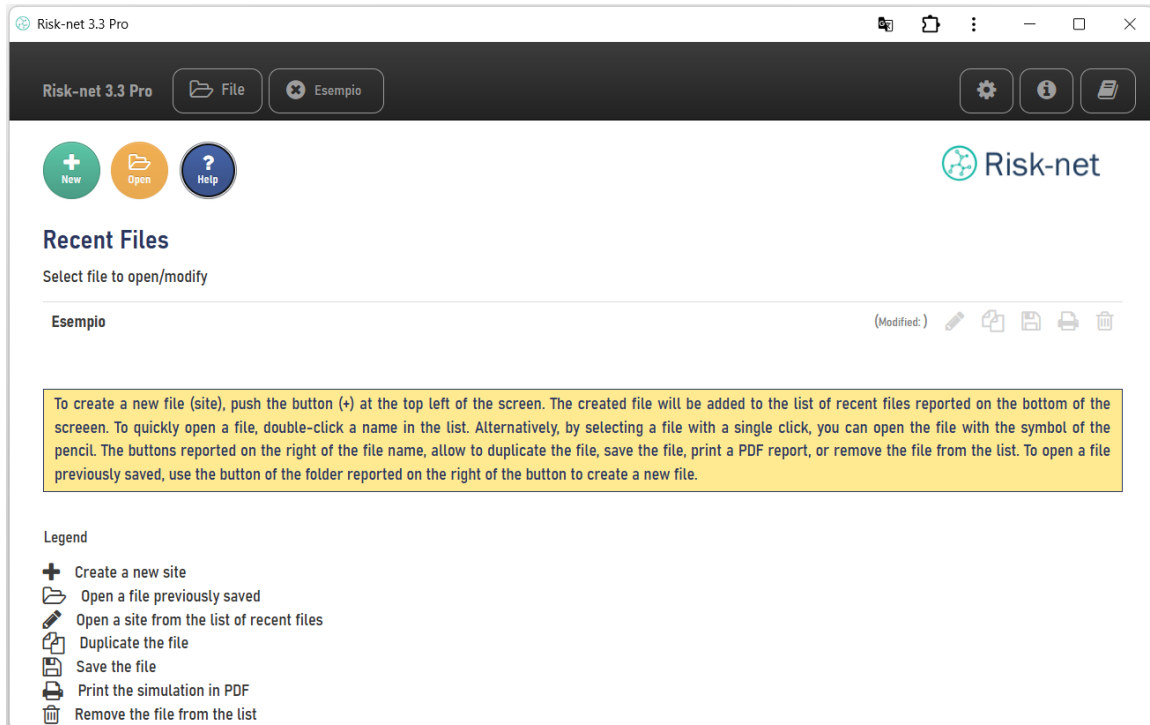











Figure 2. Main screen of the software Risk-net.

It should be noted that the software automatically saves up to five files in the internal memory. This feature helps prevent data loss in case of accidental program closure. The automatic save function applies to the five most recent files; therefore, it is recommended to save files locally on the device using 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, the font 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 3. To return to the main screen, simply click on the "File" button at the top left.

Main Screen

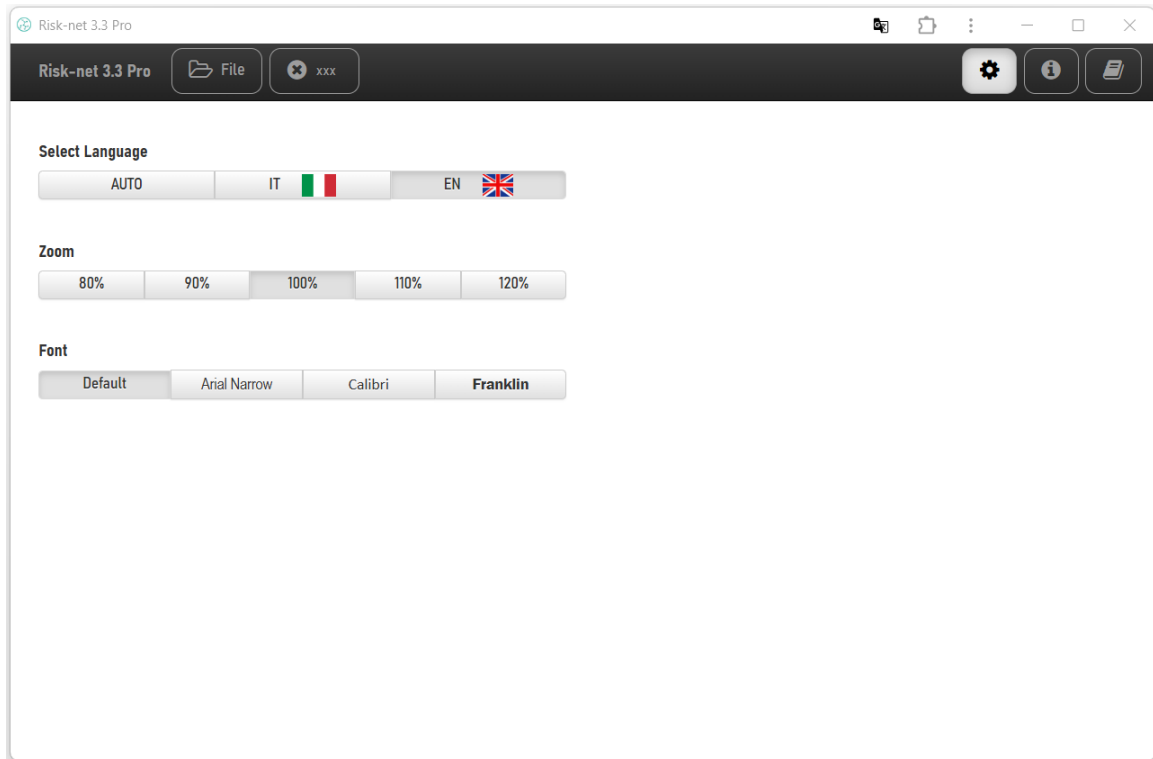



Figure 3. Main Settings.

SIMULATION SCREEN

When a new file is opened, the user is taken to the screen shown in Figure 4. From this screen, the lateral menu allows quick access to the various input and output sections. When using the software on computers or devices with small screens, the side menu can be collapsed using the button  located at the bottom right of the menu. In this mode, the navigation menu is reduced to icons only, as shown in Figure 4. The menu can be expanded again by pressing the same button.

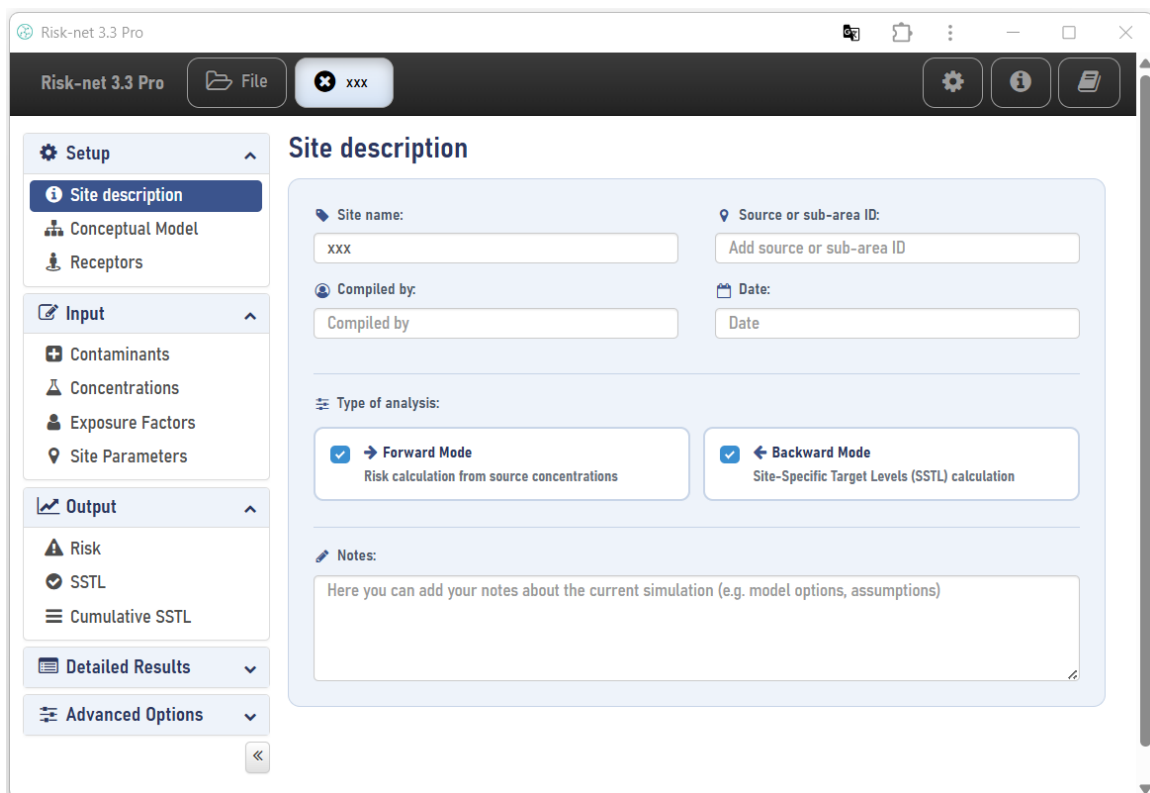


Figure 4. Simulation screen with activated lateral menu.

The menu can be expanded again by pressing the button .

Simulation Screen

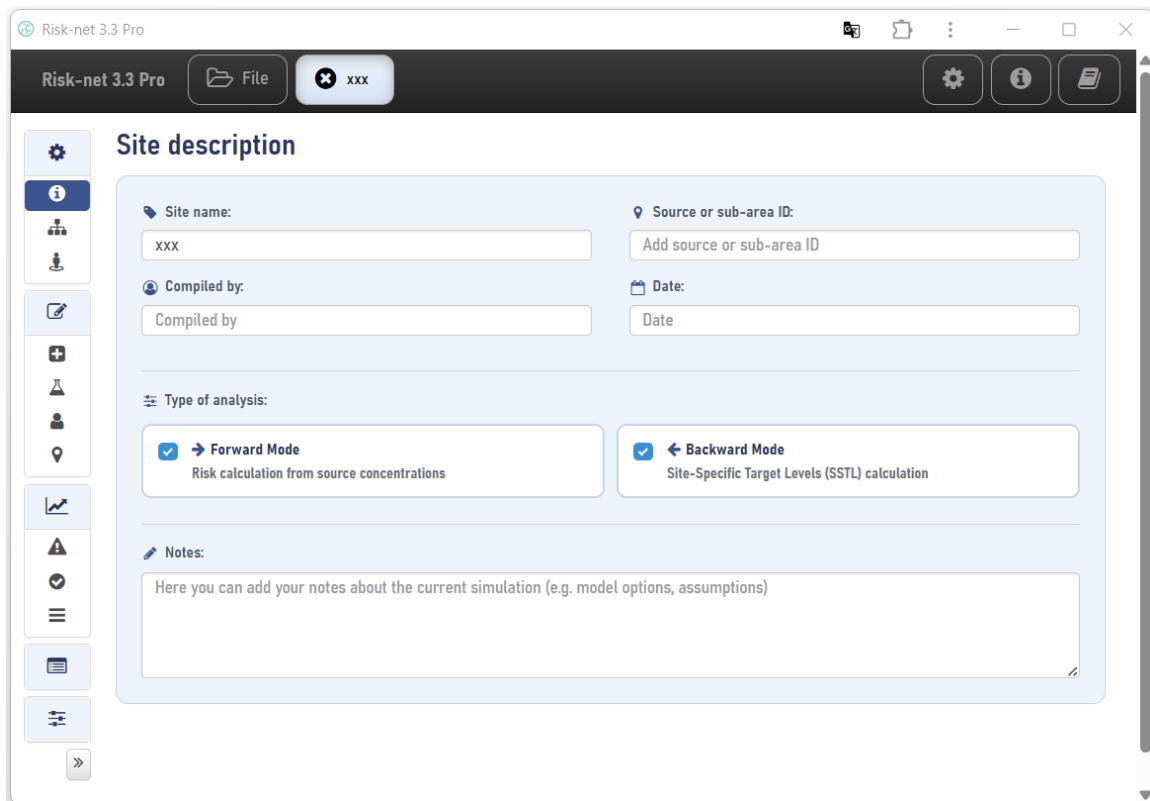



Figure 5. Simulation screen without lateral menu.

The software allows multiple simulation files to be opened simultaneously, as shown in Figure 6. In this case, the user can switch between simulation files by clicking on the corresponding tab at the top of the screen. To close a simulation file, simply click the button  displayed to the right of the file name.

Please note that simulation files are automatically saved in the recent files list; therefore, closing a file does not result in data loss. To save a file locally on the computer, the user must return to the main screen by clicking the “File” button at the top left of the interface and follow the instructions described in the previous section.

Simulation Screen

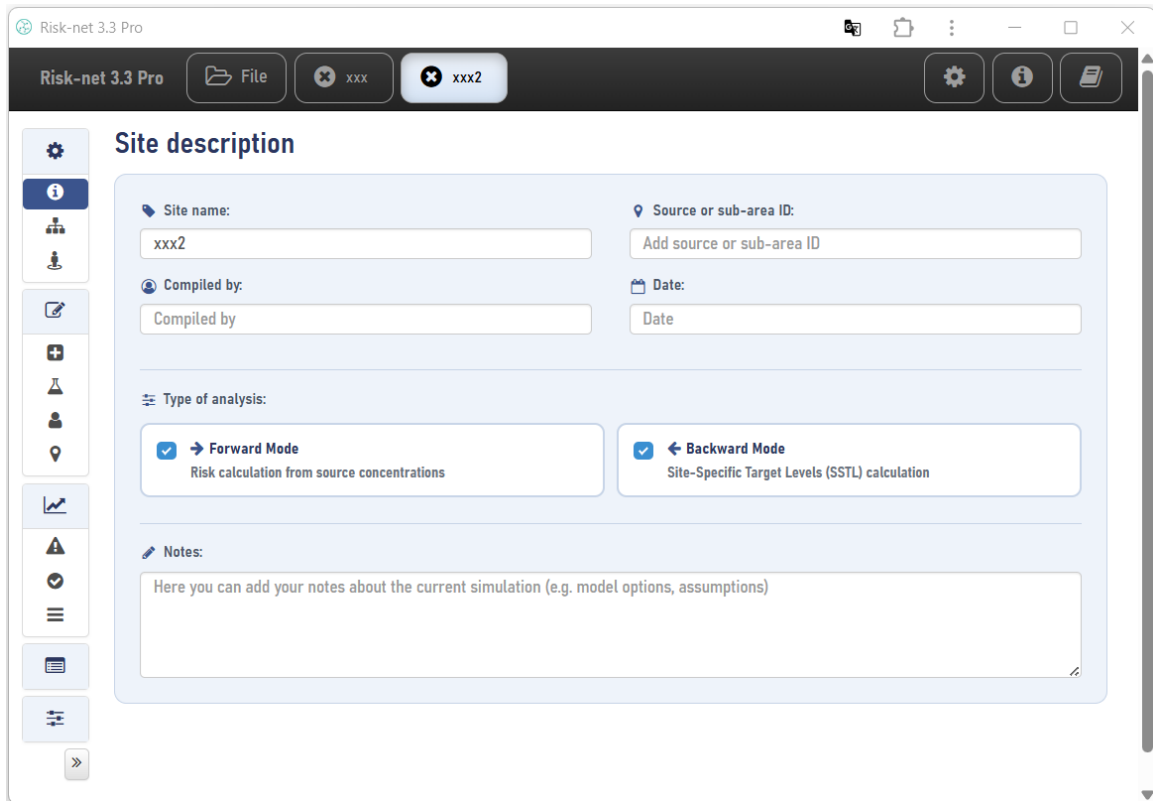


Figure 6. Multiple files open.

SIMULATION SETUP

SITE DESCRIPTION

This screen (Figure 7) is accessed by clicking “Site description” in the “Setup” menu.

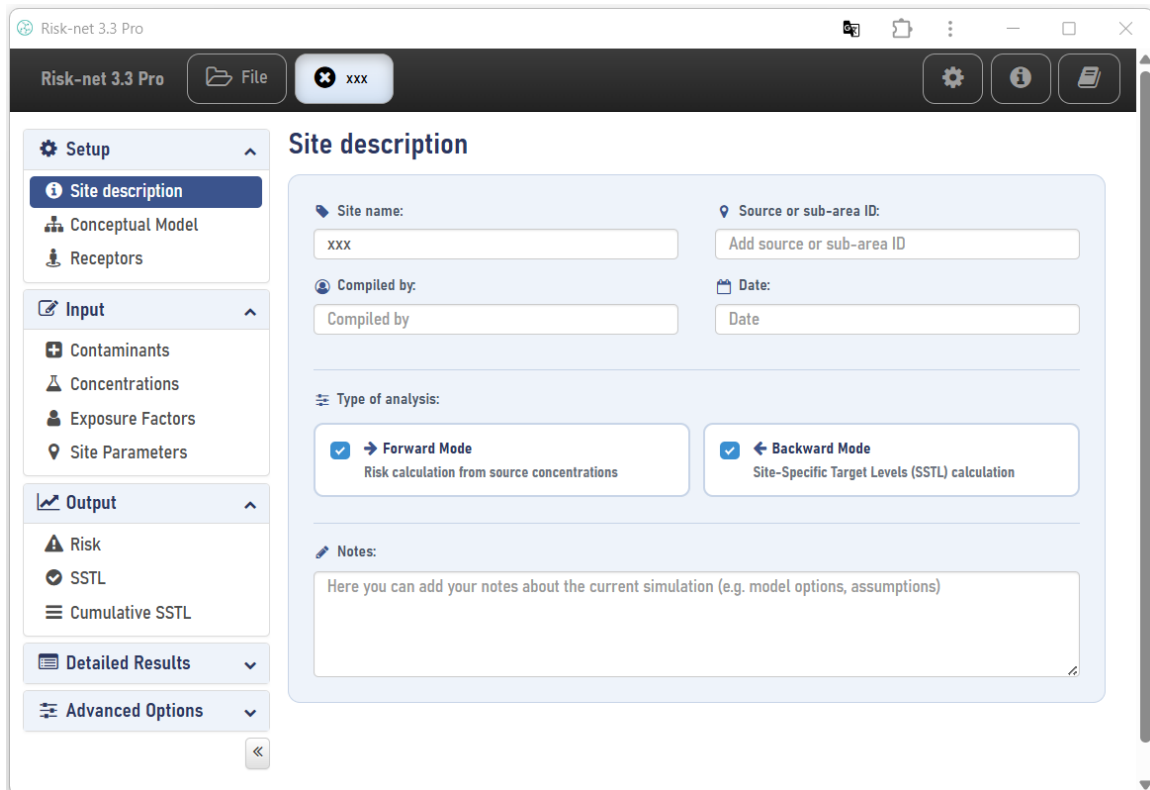


Figure 7. Site description.

On this screen, the user can define the general information of the project, including the site name, the name of any sub-area, the date, and the author (“Compiled By”). It should be noted that, in the list of temporary files, the simulation name is automatically generated based on the “Name of the site” and the sub-area name (shown in brackets) defined on this screen.

The “Notes” field allows the user to add comments related to the project. This screen also allows the user to select the type of analysis to be performed. In particular, the user can choose to perform only forward analysis for risk calculation, only backward analysis for the determination of clean-up levels, or both.

If one of the two analysis modes (forward or backward) is disabled, the corresponding output screens (Risks and/or SSTLs) will not be displayed.

CONCEPTUAL SITE MODEL

This screen (Figure 8) is accessed by clicking "Conceptual Site Model" on the "Setup" menu.

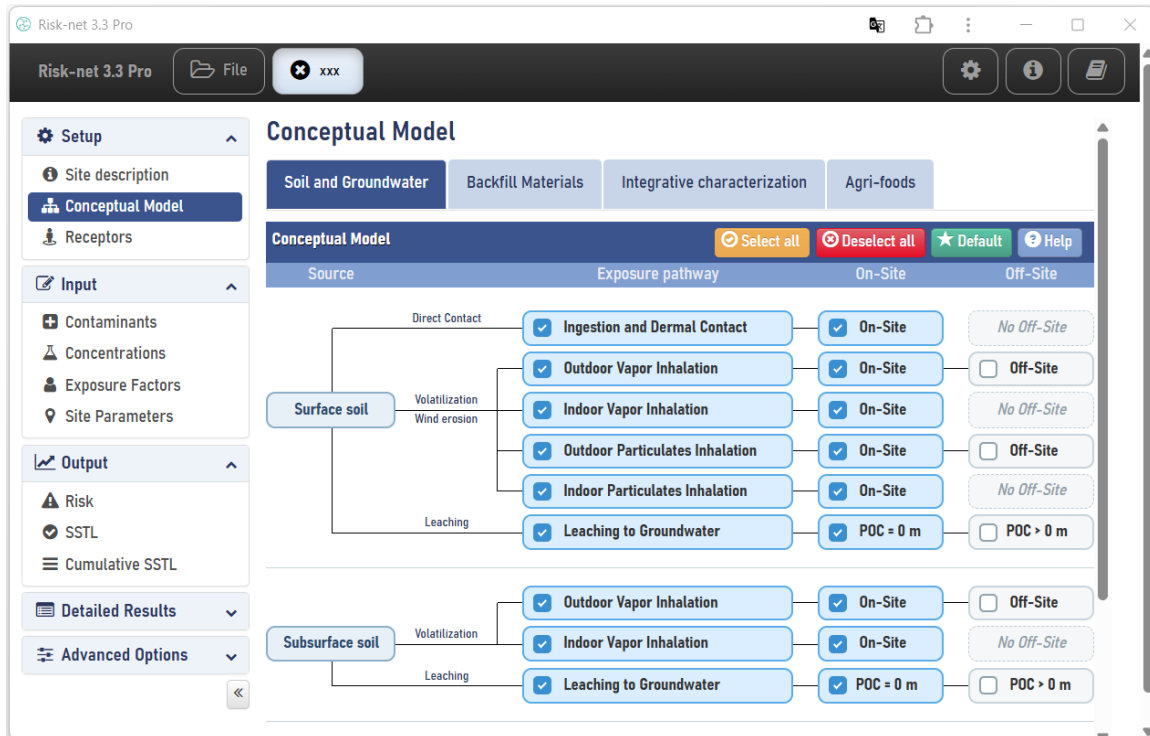


Figure 8. Conceptual Site Model.

On this screen, the user must define the exposure scenario by selecting the contaminated media, the relevant fate and transport pathways (if any), and the associated exposure routes. In particular, the user should identify the pathways that are likely to be complete, based on knowledge of the location of contaminated soil or groundwater and the position and habits of potential receptors exposed to the chemicals of concern.

Risk and SSTLs can be calculated for the following secondary sources: surface soil (0–1 m below ground level), subsurface soil (>1 m), and groundwater. For each matrix, the user must first activate the relevant exposure or migration pathways and then specify the receptor type (on-site, off-site, or both).

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

Surface Soil

- 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 directly above the source zone, whereas “off-site” refers to a receptor located at any point away from the source zone.

The checkboxes corresponding to the selected exposure pathways and receptors are highlighted in blue when activated. If an exposure pathway is selected without activating any associated receptor, it is highlighted in orange, indicating an incomplete conceptual site model.

With regard to leaching and groundwater resource protection, the term POC shown on the screen refers to the point of compliance. If the option “POC = 0 m” is selected, the risk to groundwater (when enabled in the Receptors screen) for leaching from surface or subsurface soil is calculated by comparing the predicted concentrations in groundwater directly below the source zone (i.e., without accounting for attenuation due to transport and dispersion) with the regulatory limit values (e.g., MCL, Maximum Contaminant Level).

Although the software allows both options (“POC = 0 m” and “POC > 0 m”) to be selected simultaneously, if both are activated, the final SSTLs for groundwater protection will be governed by the results corresponding to “POC = 0 m”. Therefore, particular attention should be paid to the selection of these options.

By clicking on the “Backfill Materials” tab the user accesses the screen shown in Figure 9. In this screen it is possible to select the migration and exposure routes active on the site for the Backfill Materials.

Simulation Setup

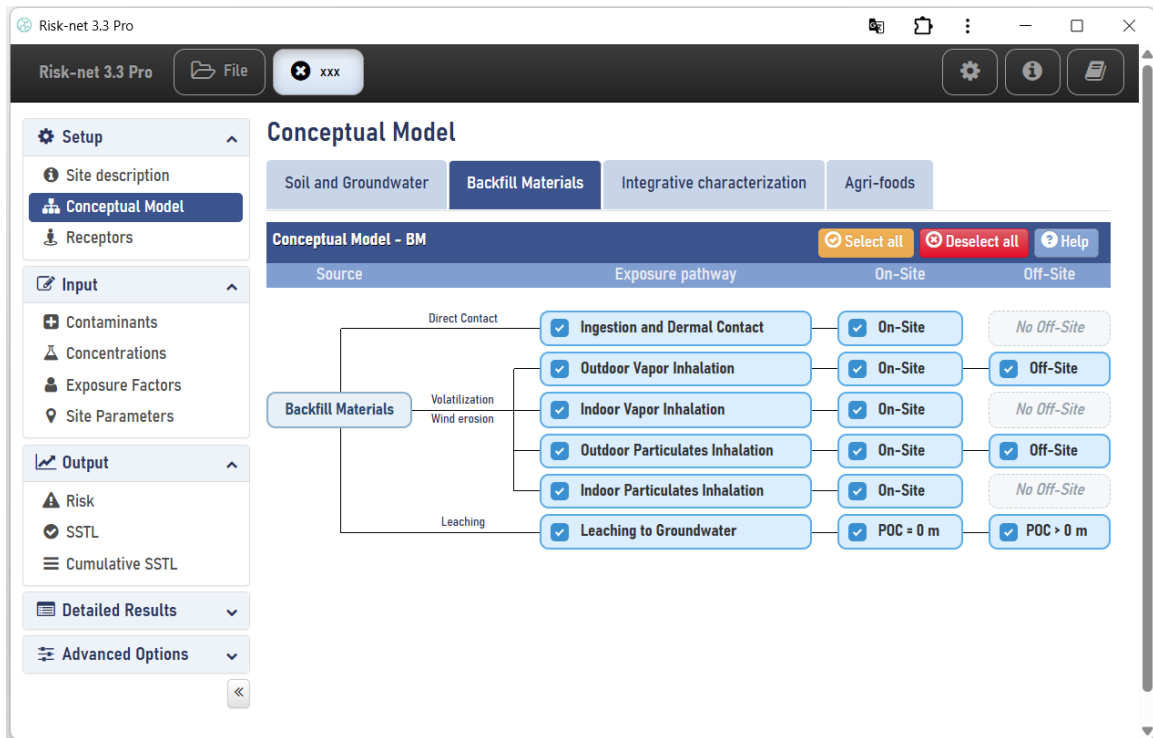


Figure 9. Conceptual model for Backfill Materials.

By clicking on the "Integrative characterization" tab the user accesses the screen shown in Figure 10. On this screen, additional monitoring data can be selected, including ambient air measurements, soil gas data, flux chamber tests, and leaching tests performed on samples collected from surface or subsurface soil.

The user must also specify whether the results of this integrative characterization are to be applied to on-site or off-site exposure scenarios.

Simulation Setup

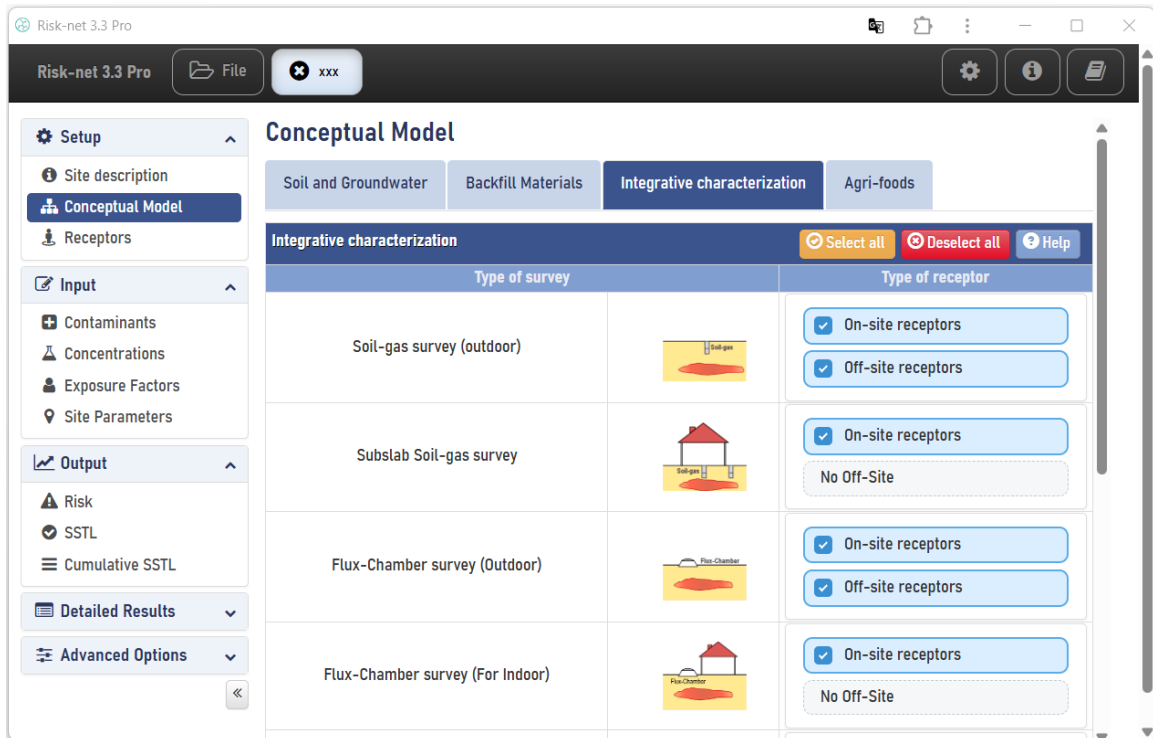


Figure 10. Integrative characterization.

By clicking on the "Agri-foods" tab the user accesses the screen shown in Figure 11. On this screen, the user can activate the risk assessment for the consumption of food products. Once the corresponding checkbox is selected, up to 10 food products can be entered. To add a product, the user must specify its name.

Simulation Setup

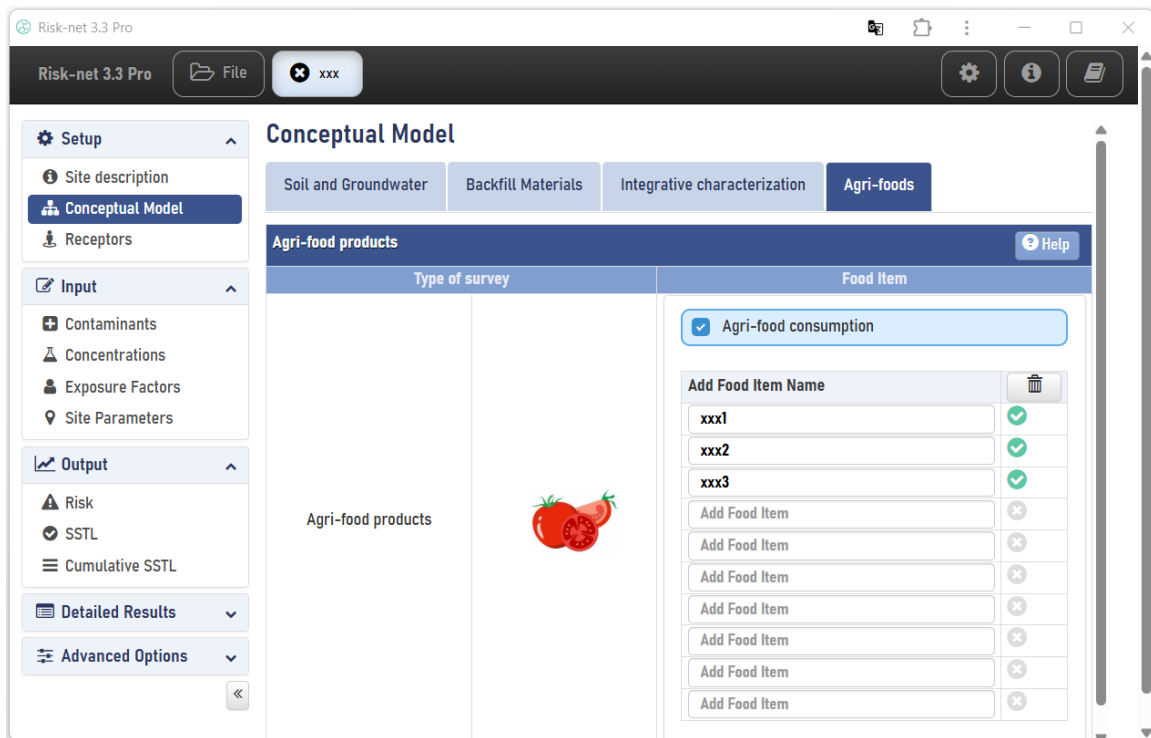


Figure 11. Agri-foods characterization.

RECEPTORS

This screen (Figure 11) is accessed by clicking "Receptors" on the "Setup" menu. On this screen, the user can select the receptors potentially exposed to contamination. The available options include:

- (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.

Note that each receptor type is defined by specific characteristics, such as body weight and skin surface area.

For carcinogenic substances, when combined receptor options are selected, the software performs an average calculation across the considered population groups. For non-carcinogenic (toxic) substances, the user can choose whether to base the assessment on a child (default option) or on the most critical receptor, depending on the selected exposure parameters.

Simulation Setup

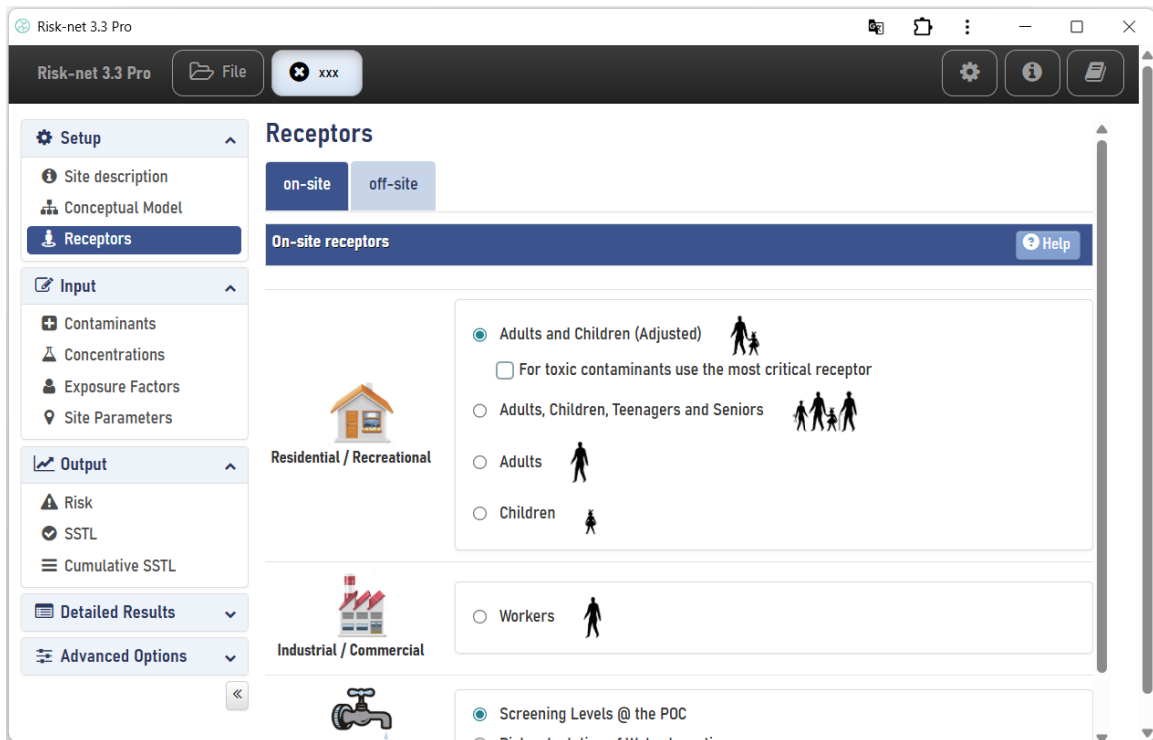


Figure 12. Receptors.

If leaching or groundwater transport is activated in the conceptual site model, the user must specify on this screen whether to evaluate the risk to the groundwater resource (i.e., by comparison with MCLs) or the health risk associated with water ingestion. These selections must be made separately for on-site and off-site receptors. Please note that if no exposure pathways are activated for either on-site or off-site receptors, the corresponding tabs will be hidden.

INPUT

CONTAMINANTS OF CONCERN

This screen (Figure 13) is accessed by clicking "Select Contaminants" on the "Input" menu.

Select Contaminants. On this screen, the user can select the chemicals of concern for the analysis. The software includes a preloaded chemical and toxicological database based on the Italian ISS-INAIL dataset.

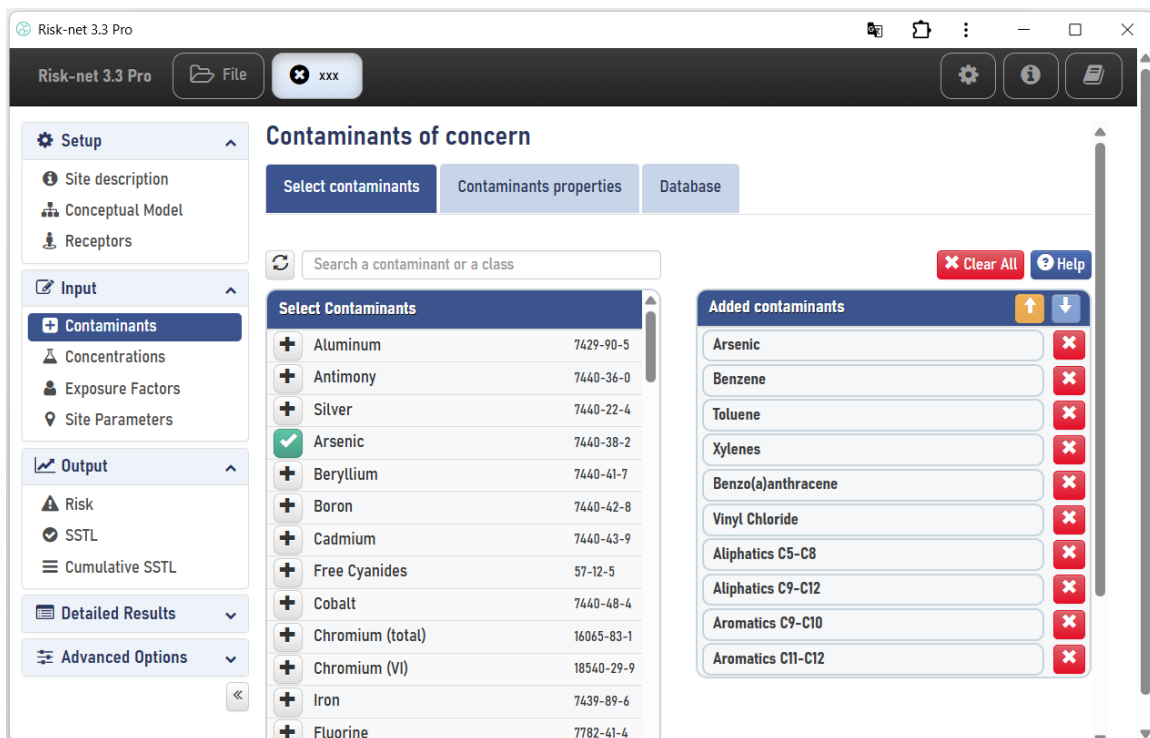





Figure 13. Select Contaminants.

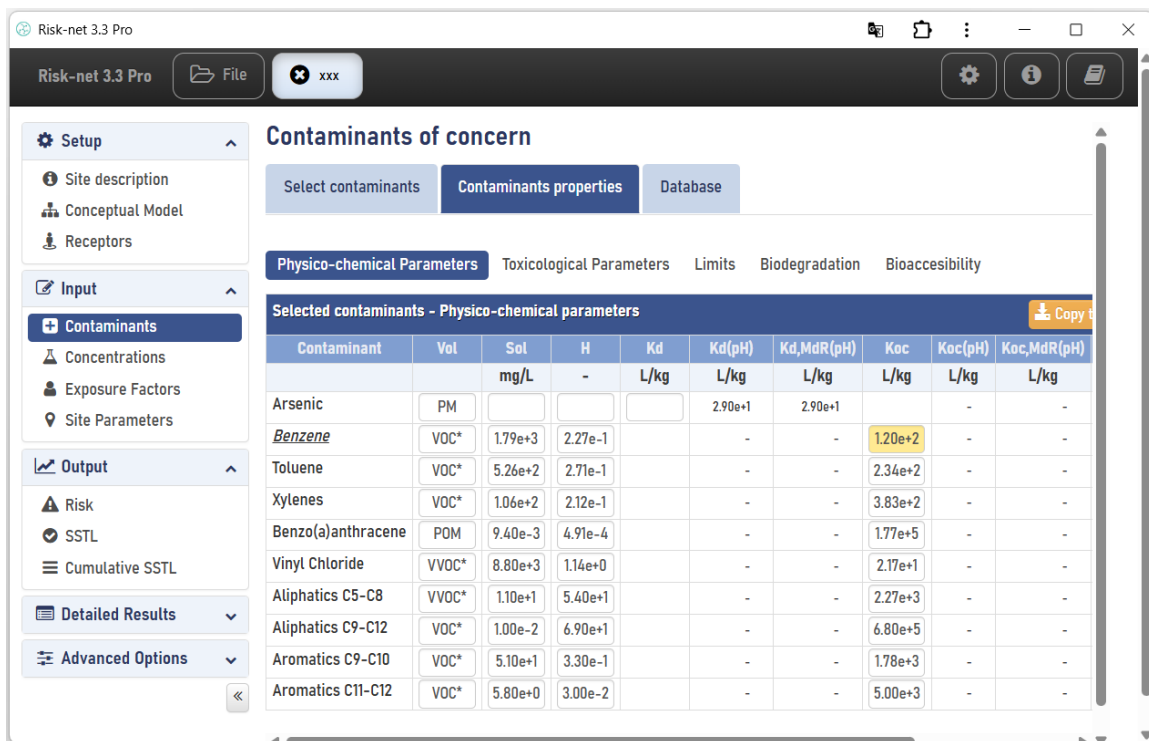
To add a chemical of concern, the user must click the **+** button located to the left of the contaminant name. Selected contaminants are highlighted with the symbol **✓**. To facilitate the selection process, the "Search for a contaminant" filter available at the top left of the screen can be used. The search can be performed not only by contaminant name, but also by CAS number, contaminant class, or volatility. The reset button **↺** allows the user to clear the applied search filter.

Input

Selected contaminants are displayed in the panel on the right side of the screen. In this section, the user can modify the order of the selected contaminants by selecting a contaminant and using the up and down arrows  , or remove individual contaminants using the corresponding button . The “Clear All” button allows all selected contaminants to be removed at once.

It should be noted that, in the current version of the software, the parameters Light Hydrocarbons (C<12), Heavy Hydrocarbons (C>12), and Total Hydrocarbons can also be selected in the absence of speciation data. In such cases, the software adopts the physicochemical and toxicological properties reported in the ISS-INAIL (2018) database, referring respectively to the MADEP classes Aromatics C9–C10 for Light Hydrocarbons, Aromatics C13–C22 for Heavy Hydrocarbons, and Aliphatics C5–C8 for Total Hydrocarbons.

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



The screenshot shows the 'Risk-net 3.3 Pro' software interface. The 'Contaminants of concern' panel is active, with the 'Contaminants properties' tab selected. The table below shows the physico-chemical parameters for selected contaminants. The 'Sol' column is highlighted in yellow for Benzene, Toluene, Xylenes, and Aromatics C9-C10. The 'Koc' column is highlighted in yellow for Benzene, Toluene, Xylenes, and Aromatics C9-C10. The 'Koc(pH)' column is highlighted in yellow for Benzene, Toluene, Xylenes, and Aromatics C9-C10. The 'Koc,MdR(pH)' column is highlighted in yellow for Benzene, Toluene, Xylenes, and Aromatics C9-C10.

Contaminant	Vol	Sol	H	Kd	Kd(pH)	Kd,MdR(pH)	Koc	Koc(pH)	Koc,MdR(pH)
		mg/L	-	L/kg	L/kg	L/kg	L/kg	L/kg	L/kg
Arsenic	PM				2.90e+1	2.90e+1	-	-	-
<i>Benzene</i>	VOC*	1.79e+3	2.27e-1		-	-	1.20e+2	-	-
Toluene	VOC*	5.26e+2	2.71e-1		-	-	2.34e+2	-	-
Xylenes	VOC*	1.06e+2	2.12e-1		-	-	3.83e+2	-	-
Benzo(a)anthracene	POM	9.40e-3	4.91e-4		-	-	1.77e+5	-	-
Vinyl Chloride	VVOC*	8.80e+3	1.14e+0		-	-	2.17e+1	-	-
Aliphatics C5-C8	VVOC*	1.10e+1	5.40e+1		-	-	2.27e+3	-	-
Aliphatics C9-C12	VOC*	1.00e-2	6.90e+1		-	-	6.80e+5	-	-
Aromatics C9-C10	VOC*	5.10e+1	3.30e-1		-	-	1.78e+3	-	-
Aromatics C11-C12	VOC*	5.80e+0	3.00e-2		-	-	5.00e+3	-	-

Figure 14. Contaminants properties.

Parameters that have been modified with respect to the default database are highlighted in yellow, and the contaminant name is displayed in italics and underlined. Please note that any changes made on this screen apply only to the current simulation. When a new simulation is started, the original database values are restored.

If biodegradation is enabled in the calculation options, the user must also define, on this

screen, the first-order biodegradation constants for the different migration pathways (volatilization, leaching, and groundwater transport).

Similarly, if bioaccessibility is considered in the calculation options for estimating soil ingestion risks, the user must specify the bioaccessible fraction for each contaminant on this screen. The bioaccessible fraction can range from 0 (non-bioaccessible contaminant) to 1 (fully bioaccessible contaminant).

Database. Here, the user can review the contaminants included in the database. By default, the software uses the Italian ISS-INAIL database (2018).

On this screen, the user can add new contaminants using the “Add contaminant” button. In this case, the database is labeled as “modified”, and user-defined contaminants are marked as “(User)”. The user can also load an external database using the “Load external DB” button. External databases must be created using the CSV file provided in the installation folder. It should be noted that an external database loaded into the software is not automatically updated if the source CSV file is modified. Therefore, if changes are made to the external database for a simulation, it must be reloaded using the same procedure.

By clicking the “Load default DB” button, the original database included in the software is restored. It should also be noted that when an external database is loaded, the automatic calculation of the partition coefficients K_{oc} and K_d as a function of site-specific pH is disabled.

On this screen, by clicking “Show DB options”, the user can select the toxicological parameters to be used for the vapor inhalation pathway. The user can choose to calculate risks and remediation targets using either reference doses (RfD for non-carcinogens and SF for carcinogens) or reference concentrations (RfC for non-carcinogens and IUR for carcinogens). The main difference between these approaches is that the method based on reference doses (RfD) accounts for body weight and inhalation rate, whereas the method based on reference concentrations (RfC) does not include adjustments based on these parameters.

The default database provided with the software is based on reference concentrations (RfC for non-carcinogens and IUR for carcinogens). Therefore, to use the reference dose approach with the default database, the user must manually provide the corresponding RfD and SF values for risk and SSTL calculations.

By default, according to the Italian ISS-INAIL database (2018), the software calculates indoor and outdoor risks only for a subset of contaminants considered sufficiently volatile. These contaminants are identified in the database with an asterisk (VVOC*, VOC*, SVOC*, VC*, and SCV*). Accordingly, the volatilization pathway is included in simulations (risk calculations and SSTLs) only for these contaminants. This option can be disabled using the checkbox available on this screen. If an external database is used, this functionality requires that volatile contaminants be properly flagged in the “Vol” column using the same notation.

Finally, to modify the physico-chemical properties of contaminants, the user must access the “Contaminants properties” screen.

Input

The screenshot shows the 'Contaminants of concern' section in Risk-net 3.3 Pro. The interface includes a sidebar with navigation options: Setup, Site description, Conceptual Model, Receptors, Input, Contaminants (selected), Concentrations, Exposure Factors, Site Parameters, Output, Risk, SSTL, Cumulative SSTL, Detailed Results, and Advanced Options. The main area displays a table of contaminants with columns for ID, Contaminant, Class, Org/Inorg, Vol, Sol, H, f(pH), Kd, Koc, and Dair. The table lists 8 contaminants, including Aluminum, Antimony, Silver, Arsenic, Beryllium, Boron, Cadmium, and Free Cyanides.

ID	Contaminant	Class	Org/Inorg	Vol	Sol	H	f(pH)	Kd	Koc	Dair
1	Aluminum	Inorganics	I	PM	-	-	-	1.50e+3	-	-
2	Antimony	Inorganics	I	PM	-	-	-	4.50e+1	-	-
3	Silver	Inorganics	I	PM	-	-	f(pH)	-	-	-
4	Arsenic	Inorganics	I	PM	-	-	f(pH)	-	-	-
5	Beryllium	Inorganics	I	PM	-	-	f(pH)	-	-	-
6	Boron	Inorganics	I	PM	-	-	-	3.00e+0	-	-
7	Cadmium	Inorganics	I	PM	-	-	f(pH)	-	-	-
8	Free Cyanides	Inorganics	I	VVC*	9.54e+4	4.15e-3	-	9.90e+0	-	2.11e-1

Figure 15. Database.

Please note that if the database is changed during an ongoing simulation, the previously selected contaminants are replaced with those having the same ID in the new database. If a previously selected contaminant is not present in the new database (i.e., no contaminant with the same ID exists), the software retains, for that contaminant, the physico-chemical and toxicological parameters from the database used in the original simulation.

Input

The screenshot displays the 'Risk-net 3.3 Pro' application window. The title bar shows 'Risk-net 3.3 Pro' and standard window controls. The interface is divided into a sidebar on the left and a main content area. The sidebar has sections for 'Setup', 'Input', and 'Output'. Under 'Input', 'Contaminants' is selected. The main content area is titled 'Contaminants of concern' and has three tabs: 'Select contaminants', 'Contaminants properties', and 'Database'. The 'Database' tab is active, showing a search bar and a table of contaminants. The table has columns: ID, Contaminant, Class, Org/Inorg, Vol, Sol, H, f(pH), Kd, and Koc. The units for Sol, H, Kd, and Koc are mg/L, -, L/kg, and L/kg respectively. A new contaminant 'Contaminant x' is highlighted in yellow, with a 'Delete' button next to it. Other contaminants listed include Aluminum, Antimony, Silver, Arsenic, Beryllium, Boron, and Cadmium.

ID	Contaminant	Class	Org/Inorg	Vol	Sol	H	f(pH)	Kd	Koc
156	Contaminant x		0	VOC*	100				100
1	Aluminum	Inorganics	I	PM	-	-		1.50e+3	-
2	Antimony	Inorganics	I	PM	-	-		4.50e+1	-
3	Silver	Inorganics	I	PM	-	-	f(pH)	-	-
4	Arsenic	Inorganics	I	PM	-	-	f(pH)	-	-
5	Beryllium	Inorganics	I	PM	-	-	f(pH)	-	-
6	Boron	Inorganics	I	PM	-	-		3.00e+0	-
7	Cadmium	Inorganics	I	PM	-	-	f(pH)	-	-

Figure 16. Example of new contaminants in the Database.

SOURCE ZONE CONCENTRATION

This screen (Figure 17) is accessed by clicking "Contaminants concentrations" on the "Input" menu. Here, the user can enter the measured concentrations for each matrix activated in the conceptual site model (CSM).

If advanced characterization data are available (e.g., eluate, soil gas, flux chamber, or air measurements) and have been enabled in the "Integrative characterization" section of the "Conceptual Model" screen, these concentrations can also be entered.

If a contaminant has been detected only in a specific medium, it can be deselected from other source media where it is not relevant by entering a value of zero. In this case, the contaminant is automatically deselected, and the green check mark to the left of its name changes to a gray "x" (as shown in the figure for Ethylbenzene in subsurface soil).

If no value is entered, the contaminant remains active, but risk calculations cannot be performed.

To import data from Excel, the user can enable the "Activate the Copy / Paste function from Excel" option available on this screen. Once enabled, the user can copy an entire column from Excel and paste it into the table by selecting the first row of the target matrix. This operation must be repeated for each source matrix activated by the user.

Contaminants for which physico-chemical and/or toxicological properties have been modified are displayed in italics and underlined.

Input

The screenshot shows the 'Representative Concentrations' input screen in Risk-net 3.3 Pro. The interface includes a sidebar menu with 'Input' selected, a top navigation bar, and a main table for entering contaminant concentrations across different media like Soil & GW, Backfill Materials, Leachate, Soil-gas, Flux Chamber, Air, and Agri-foods. A table of concentrations is shown with columns for Contaminant, Surface soil, Subsurface soil, and Groundwater, and rows for various contaminants like Arsenic, Benzene, Toluene, etc.

Contaminant	Surface soil		Subsurface soil		Groundwater	
	Soil concentration		Soil concentration		Water concentration	
	(mg/kg)	(mg/kg)	(mg/kg)	(mg/L)	(µg/L)	
Arsenic	55	110	1			
Benzene	30	60	3			
Toluene	85	170	5			
Xylenes	110	220	0.1			
Benzo(a)anthracene	200	0	0.2			
Vinyl Chloride	0	0	0.05			
Dichloromethane	30	60	0.01			

Figure 17. Source Concentration.

For concentrations in groundwater and eluate, the user can choose to enter values in either µg/L or mg/L; the software will automatically convert them to the units required for the calculations.

Similarly, concentration data for soil gas, flux chambers, and air can be entered in either µg/m³ or mg/m³.

EXPOSURE FACTORS

This screen (Figure 17) is accessed by clicking "Exposure Factors" on the "Input" menu. On this screen, the user must enter the appropriate exposure factors for each complete pathway. By default, this section includes values derived from the Italian guidelines (ISPRA, 2008).

Different columns are provided to represent the various receptor types that can be modeled in the software. These receptor types enable the calculation of baseline risks and cleanup levels based on specific physical characteristics (e.g., body weight, skin surface area) and exposure parameters (e.g., soil ingestion rate, inhalation rate).

Input

The screenshot shows the 'Exposure Factors' input screen in Risk-net 3.3 Pro. The interface is divided into a sidebar on the left and a main data entry area. The sidebar contains sections for 'Setup', 'Input', and 'Output'. The 'Input' section is active, showing options like 'Select contaminants', 'Concentrations', 'Exposure Factors', and 'Site Parameters'. The main area is titled 'Exposure Factors' and has tabs for 'on-site', 'off-site', and 'Agri-food products'. Below the tabs is a table with columns for 'Exposure Scenario' and 'On Site' (Residential, Industrial). The table lists various parameters with their symbols and units, and input fields for different receptor groups: Children, Teenagers, Adults, Seniors, and Worker. Some cells are highlighted in yellow, indicating modified values. Buttons for 'Default', 'Copy table', and 'Help' are visible at the top right of the table area.

Figure 18. Exposure Factors.

To streamline the data entry process, the software requires only the parameters that are relevant to the specific case, based on the selected exposure pathways and receptors. In particular, grey cells indicate parameters that are not required, while white cells identify the fields to be completed. Modified values are highlighted in yellow.

The “Default” button allows the user to restore the default values provided 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	cm ²	2800	2800	5700	5700	3300
Soil Dermal adherence factor	AF	mg/cm ² /d	0.2	0.2	0.07	0.07	0.2
Outdoor Vapors and Dust inhalation							
Outdoor Daily Frequency (c)	EF _{no}	h/d	24	0.5	24	1.9	8

Input

Scenario			Residential				Industrial
Exposure Parameters	Symbol	UM	Children	Teenagers	Adults	Seniors	Worker
Outdoor Daily Frequency	EFgo	h/d	24	0.5	24	1.9	8
Outdoor Vapor Inhalation rate	Bo	m ³ /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	m ³ /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 17) is accessed by clicking “Site Parameters” in the “Input” menu. In this section, the user provides the site-specific parameters required for the application of the selected fate and transport models. In particular, the following parameters must be defined:

- a) Source Geometry: geometry of the source in soil and groundwater.
- b) Vadose zone: soil properties, rainfall, infiltration rate, fraction of organic carbon, pH, etc.
- c) Backfill Materials: properties of backfill materials, 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, air dispersion, particulate emissions, etc.
- f) Indoor: building characteristics, air exchange rate, indoor/outdoor pressure differential, etc.
- g) Soil-gas and Flux Chambers: probe depth, chamber surface, etc.

By default, the software includes values derived from the Italian ISPRA guidelines (2008). To streamline the data entry process, only the parameters relevant to the specific case are required, based on the selected exposure pathways and receptors. In particular, grey cells indicate parameters that are not required, while white cells identify the fields to be completed. Modified values are highlighted in yellow.

The screenshot shows the 'Site Parameters' configuration window in Risk-net 3.3 Pro. The window has a dark header with 'Risk-net 3.3 Pro' and a 'File' menu. A sidebar on the left contains navigation options: Setup, Site description, Conceptual Model, Receptors, Input (selected), Select contaminants, Concentrations, Exposure Factors, Site Parameters (selected), Output, Risk, SSTL, Cumulative SSTL, Detailed Results, and Advanced Options. The main content area is titled 'Site Parameters' and has tabs for Source Geometry, Vadose Zone (Soil), Backfill Materials, Saturated Zone, Outdoor, and Indoor. The 'Source Geometry' tab is active, showing a table with columns for Description, Symbol, Default, Site-Specific, UM, and check. The table is divided into sections: 'Source Geometry' (with a checked 'Same dimension for all sources' checkbox), 'Surface soil', and 'Subsurface soil'. Parameters include width of source area (W, Sw, W', Sw'), ambient air mixing zone height (δ_{air}), depth to surface soil source ($L_{s,SS}$), thickness of unsaturated surface soil source (d), and depth to subsurface soil source ($L_{s,SP}$). Default values are 45, 45, 2, 45, 45, 0, 1, and 1 respectively. Site-specific values are 50, 50, 2, 45, 45, 0, 1, and 1. Units are 'm' for all. Checkmarks are present in the 'check' column for all parameters.

Description		Symbol	Default	Site-Specific	UM	check
Source Geometry						
Define source geometry in the soil <input checked="" type="checkbox"/> 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	50	m	✓
Ambient air mixing zone height		δ_{air}	2	2	m	✓
Width of source area parallel to wind direction		W'	45	45	m	✓
Width of source area orthogonal to wind direction		Sw'	45	45	m	✓
Surface soil						
Depth to surface soil source		$L_{s,SS}$	0	0	m	✓
Thickness of unsaturated surface soil source		d	1	1	m	✓
Subsurface soil						
Depth to subsurface soil source		$L_{s,SP}$	1	1	m	✓

Figure 19. Site Parameters.

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

Same dimension for all sources. By default, the software assumes the same source geometry for all source media selected in the conceptual site model (e.g., surface soil, subsurface soil, and groundwater). If the source dimensions differ, the user can deselect the “Same dimension for all sources” checkbox. In this case, specific geometric parameters can be defined for each environmental compartment.

Lens present. By activating this option, the user can account for the presence of a geological vapor barrier (e.g., a clay lens) located between the contamination source and the ground surface in the calculation of risks and SSTLs for indoor and outdoor volatilization from subsurface soil and groundwater. When enabled, the user must define the thickness, porosity, and water content of the lens, which are used to estimate molecular diffusion through this layer (see Appendix for details).

Soil texture. The user can select the predominant soil texture from a drop-down menu and use the default values provided by the ISPRA guidelines (2008) or enter site-specific data by selecting the “Site-specific” option. Table 3 reports the default values implemented in the software as a function of soil texture. The software also includes a USDA-based tool to determine soil texture: by clicking the “USDA” button, the user can input the percentages of sand and silt (with clay calculated by difference), and then click

Input

“Calculate USDA class” to identify the corresponding texture. The calculated class can be selected using the “Select calculated class” button.

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

Soil Infiltration Rate. The user can choose to calculate this parameter based on rainfall and soil type using empirical equations from the ISPRA guidelines (2008), or to enter it manually (see Appendix for details).

HDPE or low-permeability layer present. This option allows the user to define the characteristics of an HDPE liner above the contamination source or a low-permeability layer between the source and the aquifer. These parameters are used to calculate the effective soil infiltration rate for the leaching pathway. The equations used are reported in the Appendix and are based on ISPRA (2005) landfill risk assessment models. These parameters are applied only to the leaching pathway and are not considered for volatilization.

Select the type of backfill materials. The user can select the type of backfill material from a drop-down menu, using default values from SNPA Guidelines 46bis/2023, or define site-specific data by selecting the “Site-specific” option. Table 4 reports the values implemented in the software for different backfill materials.

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

Input

Backfill Material	K_{sat}	θ_r	θ_e	θ_a	θ_w	ρ_{MdR}	pH_{MdR}
	m/s	-	-	-	-	kg/L	-
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 backfill-related pathways are activated in the conceptual model, the user can enable the “Use Backfill Material Parameters” option in the “Backfill Materials” screen. This allows the use of capillary fringe and unsaturated zone parameters defined for backfill materials in the calculation of diffusion coefficients for volatilization (both indoor and outdoor) from groundwater. This option is relevant when backfill materials significantly influence the unsaturated zone near the saturated zone.

Effective infiltration calculation in Backfill Materials. By activating the “Consider l_{eff} used for soils” checkbox, the user can apply the effective infiltration value estimated for soils. According to SNPA Guidelines 46bis/2023, this option should be used when less permeable layers are present within, above, or below the backfill materials, with sufficient thickness and spatial continuity in the unsaturated zone.

Selection of Saturated Zone Texture. Based on site-specific conditions, the user can select the soil type in the saturated zone using default values from ISPRA (2008), as referenced in SNPA Guidelines 46bis/2023 (in the presence of backfill materials) or define site-specific data. Table 5 reports the values implemented in the software.

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

Input

Texture	K _{sat}	θ _e
	m/s	-
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 either enter dispersivity values manually or calculate them based on the distance to the point of compliance (see Appendix for details).

Calculate wind speed. The wind speed entered into the software should refer to the height of the air mixing zone (default: 2 m above ground level). If available data refer to a different height (e.g., 10 m), the software allows recalculation using empirical equations provided in the ISPRA guidelines (see Appendix).

Air dispersion coefficients. These can be entered manually or calculated based on atmospheric stability class and the distance to off-site receptors, using the empirical equations proposed by Briggs (1973).

Pressure difference between outdoor and indoor. If convective vapor transport into indoor environments is relevant, the user must enter a value of Δp greater than zero and provide the additional required parameters.

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

Empirical soil-gas attenuation factor of soil-gas. For soil-gas data, instead of using the analytical models implemented in the software, the user can activate this option to input empirical attenuation factors for calculating risks associated with indoor and outdoor vapor inhalation pathways.

MODEL OPTIONS

By default, Risk-net implements the equations and calculation criteria defined in the Italian ISPRA guidelines (2008). However, to enhance the flexibility of the tool, additional calculation options can be activated and customized.

To view or modify these options, the user must access the “Model options” section from the “Advanced Options” menu (Figure 19). The available settings are organized into the following tabs: “Volatilization”, “Leaching”, “Groundwater dispersion”, “Csat”, “Exposure”, and “Limits”.

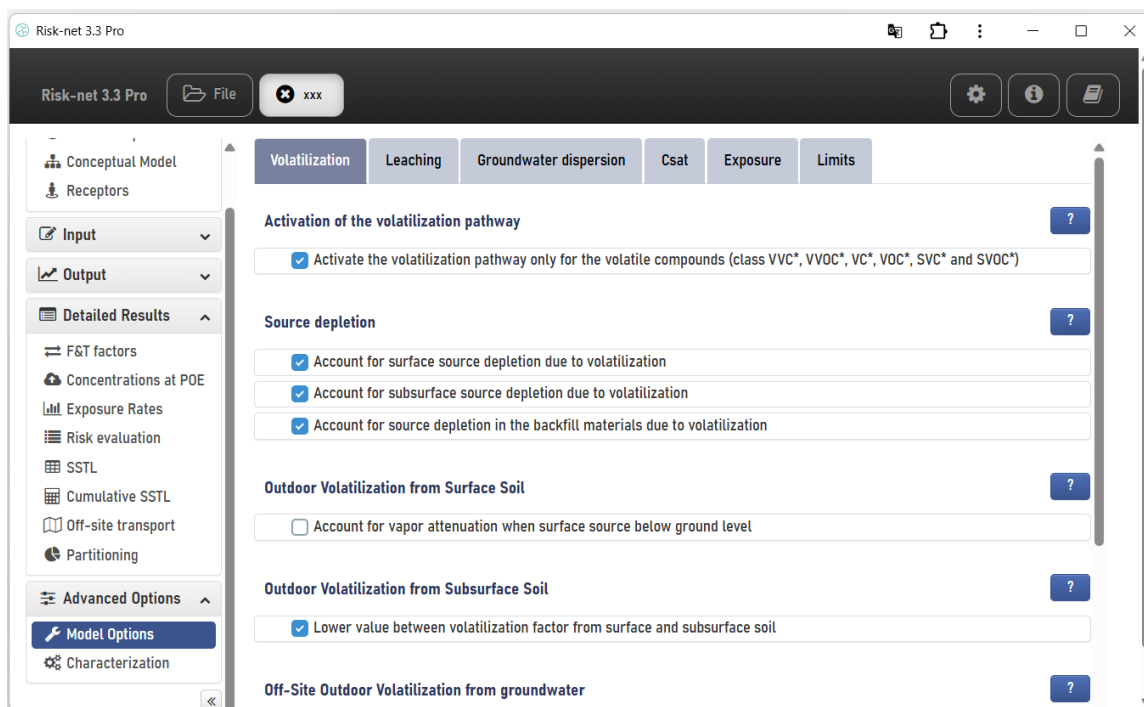


Figure 20. Site Parameters.

The different options are briefly described below.

VOLATILIZATION

Source depletion. By activating this option, the software accounts for source depletion through a mass balance approach. In particular, outdoor and indoor volatilization are calculated, for each contaminant, by selecting the lower value between the fate and

Model options

transport factor and the mass balance estimate. Further details are provided in the Appendix.

Outdoor Volatilization from Surface Soil. When this option is enabled, if the contamination source in surface soil is located below ground level, the volatilization factor is calculated using the subsurface soil model.

Outdoor Volatilization from Subsurface Soil. When activated, the software compares the volatilization estimated for subsurface soil with that estimated for surface soil and selects the lower value as representative.

Off-Site Outdoor Volatilization from groundwater. For contaminated groundwater, off-site vapor transport can be modeled either as volatilization from the source followed by atmospheric dispersion (ADF), or as groundwater transport (DAF) followed by volatilization.

Biodegradation during volatilization. This option allows the user to account for aerobic biodegradation of vapors in the subsurface. In this case, the biodegradation rate constant must be defined in the chemical properties screen, and the thickness of the aerobic zone must be specified in the site parameters screen.

LEACHING

Source depletion. When activated, the software accounts for source depletion using a mass balance approach. The leaching factor is calculated, for each contaminant, as the lower value between the fate and transport factor and the mass balance estimate.

Soil Attenuation Model (SAM). The SAM (Connor, 1997) adjusts the equilibrium soil leachate concentration to account for sorptive mass loss as leachate percolates toward groundwater. The contaminated soil is treated as a finite source mass, and infiltrating water redistributes this mass throughout the thickness of the soil column before reaching groundwater.

Biodegradation during leaching to groundwater. This option accounts for biodegradation during leaching in the unsaturated zone. The biodegradation rate constant must be defined in the chemical properties screen.

GROUNDWATER DISPERSION

Groundwater Dispersion. The user can select the dispersion model based on site conditions. Dispersion can be simulated considering full three-dimensional dispersion (DAF1), longitudinal and transverse dispersion with downward vertical dispersion (DAF2), or only longitudinal and transverse dispersion without vertical dispersion (DAF3). The corresponding equations are reported in the Appendix.

Check on the groundwater mixing zone height. When activated, the software automatically applies the DAF3 model if the calculated mixing zone thickness coincides with the aquifer thickness.

Biodegradation during groundwater transport. This option allows biodegradation during contaminant transport in groundwater to be considered. The biodegradation rate constant must be defined in the chemical properties screen.

CSAT

Saturation Concentration (C_{sat}). When activated, the software calculates the soil saturation concentration (C_{sat}), corresponding to the maximum concentration at which the contaminant reaches solubility in the dissolved phase and vapor pressure in soil gas. For indirect exposure pathways (volatilization and leaching), if the source concentration exceeds C_{sat}, risks are calculated using the solubility and vapor pressure limits. For direct exposure pathways (soil ingestion and dermal contact), concentrations above C_{sat} do not affect risk estimates, as exposure to a separate phase may occur.

For clean-up levels, if calculated SSTLs exceed C_{sat}, the output indicates "> C_{sat}" rather than reporting the numerical value. This condition implies that, even at maximum solubility or volatilization potential, risks remain below acceptable thresholds (e.g., R = 10⁻⁶ or HI = 1).

If the C_{sat} option is deactivated, a sub-option allows verification of C_{sat} only during SSTL calculation and not during direct risk calculation. Although this may lead to inconsistencies between risk and SSTL results, it is included to replicate the behavior of other tools (e.g., RBCA ToolKit).

Source depletion. When activated, the mass balance used to estimate source depletion accounts for the presence of any separate phase in the subsurface.

Model options

EXPOSURE

Adjustment factor for carcinogenic parameters of children (ADAF). When activated, the software applies an adjustment factor (ADAF) to carcinogenic toxicological parameters for child receptors. ADAF values can be modified in the toxicological parameters screen.

RfD vs RfC. For the inhalation pathway, the user can choose between two approaches: one based on reference doses (RfD and SF), which accounts for body weight and inhalation rate, and one based on reference concentrations (RfC), which does not include such adjustments.

Bioaccessibility. When activated, the software accounts for the bioaccessible fraction in soil ingestion risk calculations. This fraction can be defined in the screen for contaminant physico-chemical properties.

LIMITS

Limits. In this section, the user can define acceptable risk levels for both individual contaminants and cumulative exposure, including carcinogenic risk and hazard index for non-carcinogenic effects.

ADVANCED SITE CHARACTERIZATION

This screen (Figure 17) is accessed by clicking "Advanced Characterization" on the "Advanced Options" menu.

Model options

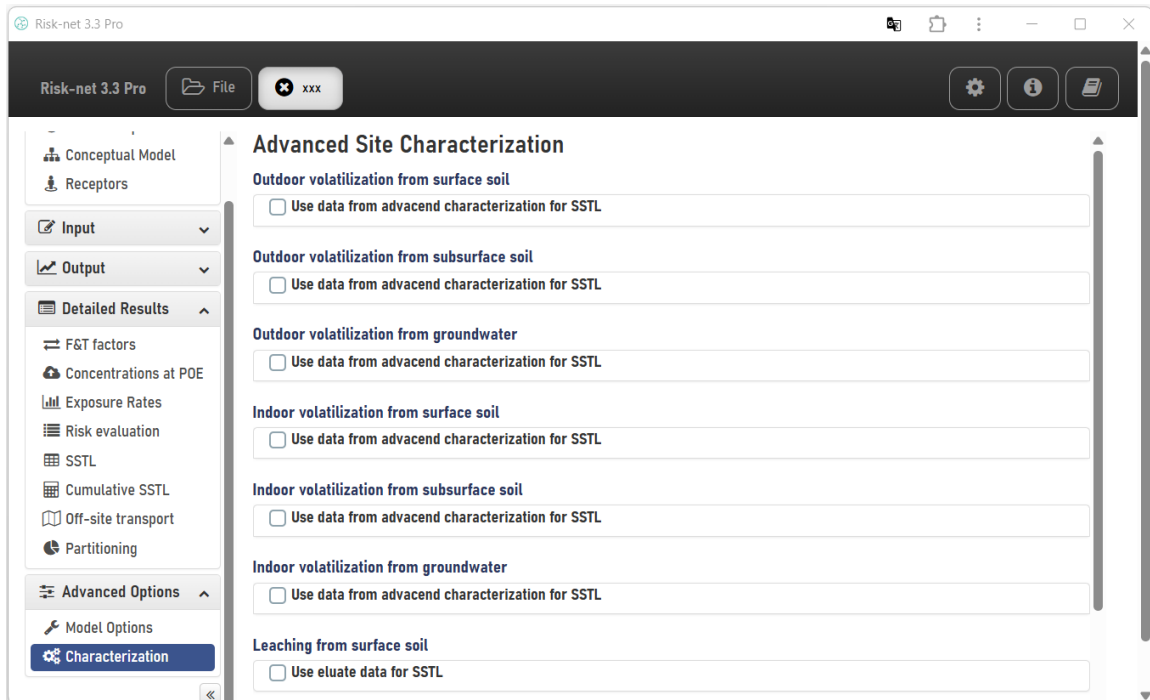


Figure 21. Advanced Site Characterization.

By default, data from advanced site characterization are used only to estimate risks to human health and the environment for the selected receptors. On this screen, the user can choose to also apply these data to the estimation of clean-up levels in surface soil, subsurface soil, and groundwater.

In this case, the data are used to derive a semi-empirical fate and transport factor, which is applied to update the clean-up levels originally calculated using mathematical models alone. For further details, please refer to the Appendix, where the implemented equations are described.

OUTPUT

RISK

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

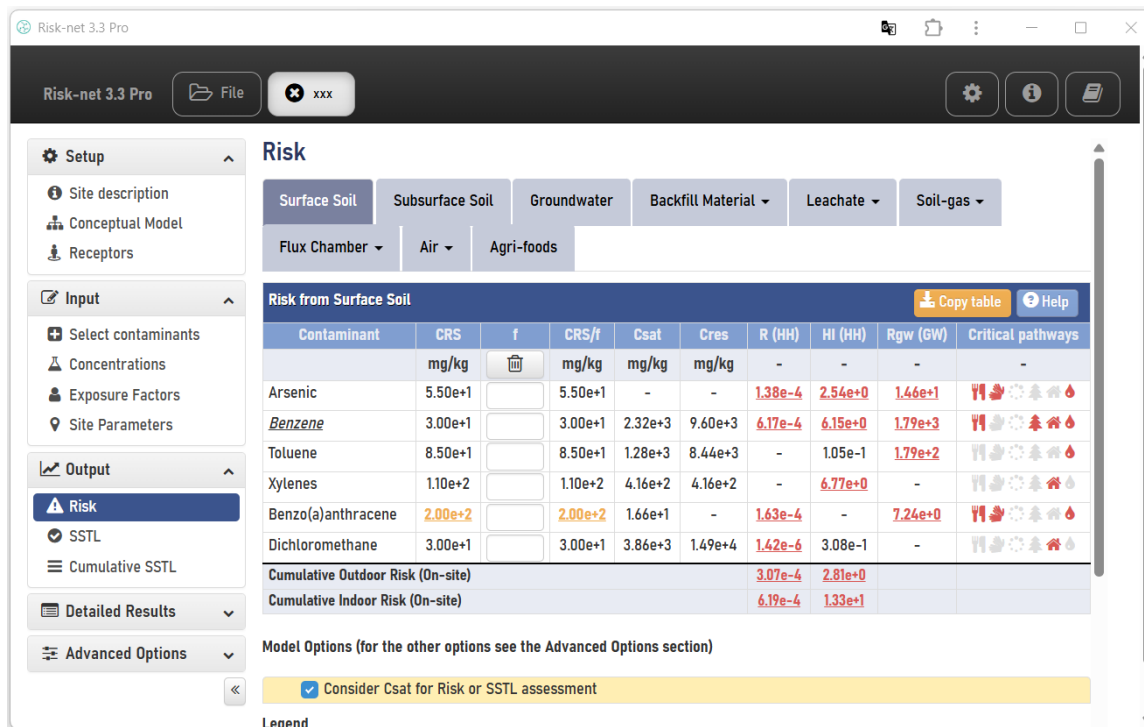


Figure 22. Baseline Risks.

This screen displays the risks to human health, including individual risk (R) for each contaminant and cumulative risk (calculated as the sum of the risks for all selected contaminants), as well as the hazard index (HI) and the risk to groundwater resources (R_{gw}), calculated for each source defined in the conceptual site model.

Risks exceeding acceptable limits are highlighted in red. In addition, the last column of the table identifies the critical exposure or transport pathways (i.e., those associated with risks above acceptable limits), also highlighted in red for each contaminant.

Source concentrations exceeding the saturation concentration (or solubility, in the case of groundwater contamination) are highlighted in yellow.

On this screen, the user can iteratively determine the source concentration that ensures acceptable risk levels by entering a correction factor for each contaminant in the "f" column.

Output

The “Copy table” command allows the user to export the results table to Word or Excel while preserving its formatting.

Contaminants for which physico-chemical and/or toxicological properties have been modified are displayed in italics and underlined.

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)
R _{gw}	Risk for the groundwater resource
C _{sat}	Saturation concentration
C _{res}	Residual Concentration (screening NAPL)
Sol	Solubility

SITE-SPECIFIC TARGET LEVELS (SSTL)

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

This screen displays the maximum acceptable concentrations in the affected source media (i.e., Site-Specific Target Levels, SSTLs) for each contaminant of concern, ensuring acceptable individual risks for human health (R and HI) and for groundwater resources (R_{gw}).

Contaminants for which the source concentration exceeds the calculated SSTL are highlighted in red. SSTLs lower than the PRG (Preliminary Remediation Goals) values defined in the database are marked with an asterisk.

Source concentrations exceeding the saturation concentration (or solubility, in the case of groundwater contamination) are highlighted in yellow.

The “Copy table” command allows the user to export the results table to Word or Excel while preserving its formatting.

Contaminants for which physico-chemical and/or toxicological properties have been modified are displayed in italics and underlined.

Output

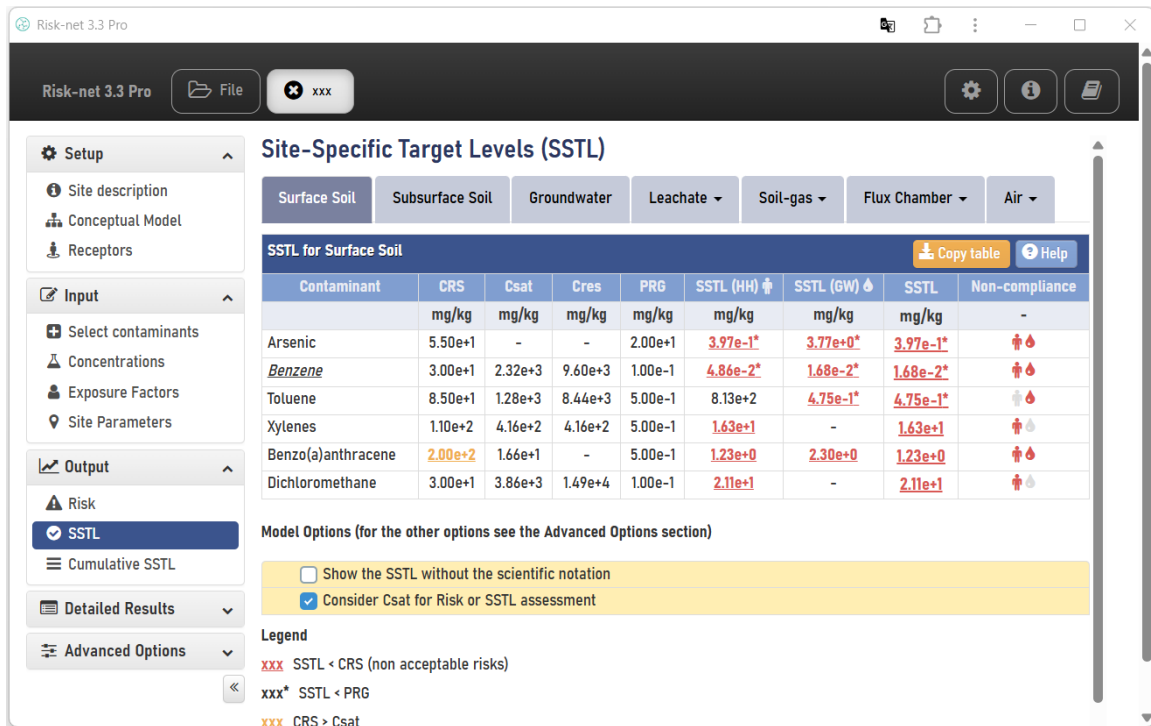


Figure 23. Site-Specific Target Levels (SSTL).

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 SSSL

This screen (Figure 24) is accessed by clicking "Cumulative SSSL" on the "Output" menu.

Cumulative SSSL

Surface Soil Subsurface Soil Groundwater Leachate Soil-gas Flux Chamber Air

Cumulative SSSL - Surface Soil Copy table Help

Contaminant	CRS	SSSLind	f	SSSLcum	PRG	Csat	R (HH)	HI (HH)	Rgw (GW)
	mg/kg	mg/kg	auto	mg/kg	mg/kg	mg/kg	-	-	-
Arsenic	5.50e+1	<u>3.97e-1*</u>		<u>3.97e-1*</u>	2.00e+1	-	1.00e-6	1.83e-2	1.05e-1
<i>Benzene</i>	3.00e+1	<u>1.68e-2*</u>		<u>1.68e-2*</u>	1.00e-1	2.32e+3	3.46e-7	3.45e-3	1.00e+0
Toluene	8.50e+1	<u>4.75e-1*</u>		<u>4.75e-1*</u>	5.00e-1	1.28e+3	-	5.85e-4	1.00e+0
Xylenes	1.10e+2	<u>1.63e+1</u>		<u>1.63e+1</u>	5.00e-1	4.16e+2	-	1.00e+0	-
Benzo(a)anthracene	<u>2.00e+2</u>	<u>1.23e+0</u>		<u>1.23e+0</u>	5.00e-1	1.66e+1	1.00e-6	-	5.35e-1
Dichloromethane	3.00e+1	<u>2.11e+1</u>		<u>2.11e+1</u>	1.00e-1	3.86e+3	1.00e-6	2.16e-1	-
Cumulative Outdoor Risk (On-site)							2.33e-6	8.05e-2	
Cumulative Indoor Risk (On-site)							1.35e-6	<u>1.22e+0</u>	

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

- Show the SSSL without the scientific notation
- For the SSSL-PRG set the SSSL equal to the PRG and exclude them from the check of the cumulative risks

Figure 24. Cumulative Site-Specific Target Levels (SSSL).

From this screen, the user can verify whether the individual SSSLs (SSSLind) calculated for each contaminant ensure acceptable cumulative risks associated with the simultaneous presence of multiple substances.

If cumulative risks are not acceptable (highlighted in blue), the user should reduce the SSSLind values until a condition is reached that satisfies both individual and cumulative risk criteria. This can be achieved by iteratively adjusting the correction factor in the "f" column until acceptable cumulative risks are obtained.

The "auto" button in the "f" column automatically assigns a correction factor equal to the number of selected contaminants, representing a conservative approach.

The adjusted SSSL (SSSL / f), which ensures compliance with both individual and cumulative risk criteria, represents the cumulative SSSL (SSSLcum).

Contaminants for which physico-chemical and/or toxicological properties have been modified are displayed in italics and underlined.

Table 8 describes the different keywords and symbols related to the calculation of the Cumulative SSSLs.

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 hydrocarbon compounds classified according to MADEP or TPHCWG are selected among the contaminants of concern, an additional table is displayed in the Cumulative SSTL screen.

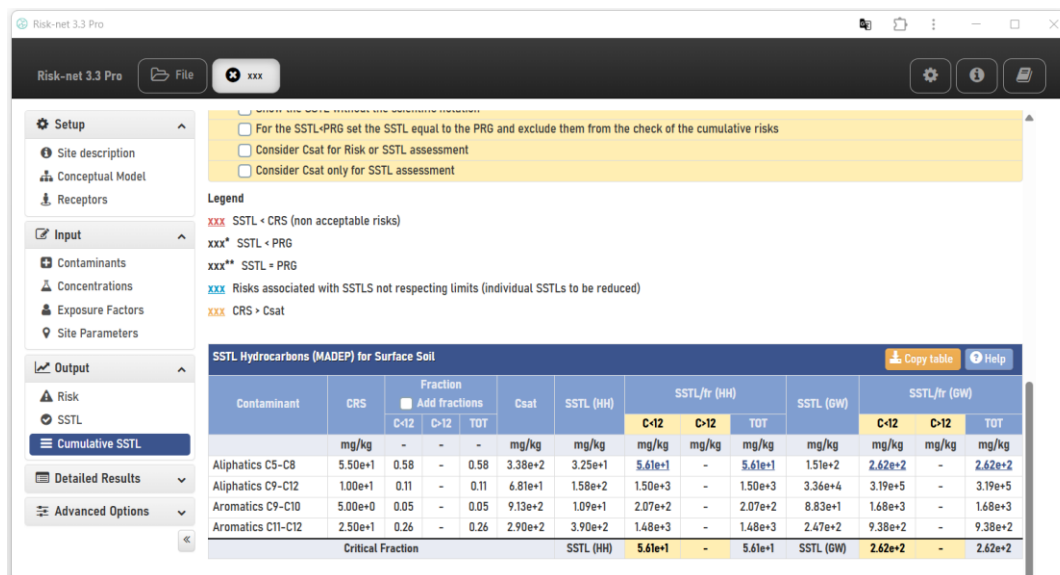


Figure 25. SSTL for TPH mixtures.

This table reports the SSTLs calculated for “Hydrocarbons C<12”, “Hydrocarbons C>12”, and “Total hydrocarbons”. This section provides the SSTLs for light hydrocarbons (C<12), heavy hydrocarbons (C>12), and total hydrocarbons (TOT), calculated using the “critical fraction” method based on the selected hydrocarbon classes. The calculation is

performed according to both MADEP and TPHCWG classifications.

The most critical fraction is identified based on the SSTL calculated for each class and its proportion within the mixture, which is estimated from the concentrations defined by the user.

For further details, please refer to the Appendix, where the implemented equations are described.

DETAILED RESULTS

In addition to the main outputs described in the previous paragraphs, the user can review in detail the results obtained at each stage of the calculations, as briefly described below.

FATE & TRANSPORT FACTORS

This screen displays the fate and transport (F&T) factors calculated for the migration pathways activated in the conceptual site model.

F&T values corresponding to the mass balance in the source (when this option is enabled in the “Model options” screen) are highlighted in yellow. Semi-empirical F&T values derived from advanced characterization data (when this option is enabled in the “Advanced characterization” screen) are highlighted in purple.

Contaminants for which physico-chemical and/or toxicological properties have been modified are displayed in italics and underlined.

F&T factors

Surface Soil Subsurface Soil Groundwater Backfill Material Leachate Soil-gas Flux Chamber Air

Fate and Transport Factors - Surface Soil Copy table

Contaminant	Dss,eff cm ² /s	Dcrack,eff cm ² /s	LF (mg/L)/(mg/kg)	VFss (mg/m ³)/(mg/kg)	VFsesp (mg/m ³)/(mg/kg)	PEF (mg/m ³)/(mg/kg)	DAF ss (mg/L)/(mg/L)	(mg/L)/(mg/L)	(mg/L)/(mg/L)
Arsenic	-	-	2.65e-3	-	-	6.90e-12	1.50e+0		
<u><i>Benzene</i></u>	7.10e-3	6.98e-3	5.95e-2	1.80e-5	6.42e-3	6.90e-12	1.50e+0		
Toluene	6.17e-3	6.07e-3	3.16e-2	1.80e-5	6.42e-3	6.90e-12	1.50e+0		
Xylenes	6.72e-3	6.61e-3	1.96e-2	1.80e-5	6.42e-3	6.90e-12	1.50e+0		
Benzo(a)anthracene	-	-	4.35e-5	-	-	6.90e-12	1.50e+0		
Dichloromethane	7.93e-3	7.80e-3	2.59e-1	1.80e-5	6.42e-3	6.90e-12	1.50e+0		

Figure 26. Fate & Transport Factors.

Detailed results

CONCENTRATIONS AT THE POINT OF EXPOSURE

This screen displays the concentrations at the point of exposure, calculated using the fate and transport factors and the source concentrations defined by the user for the migration pathways activated in the conceptual site model. Contaminants for which physico-chemical and/or toxicological properties have been modified are displayed in italics and underlined.

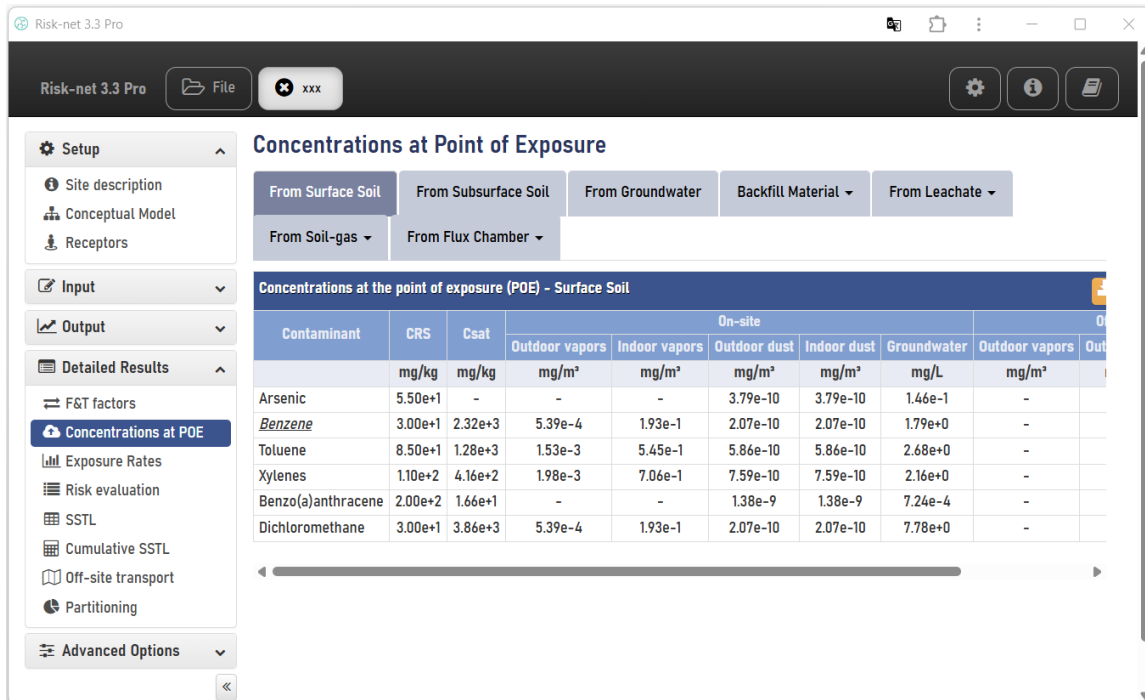


Figure 27. Concentration at the point of exposure.

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.

Detailed results

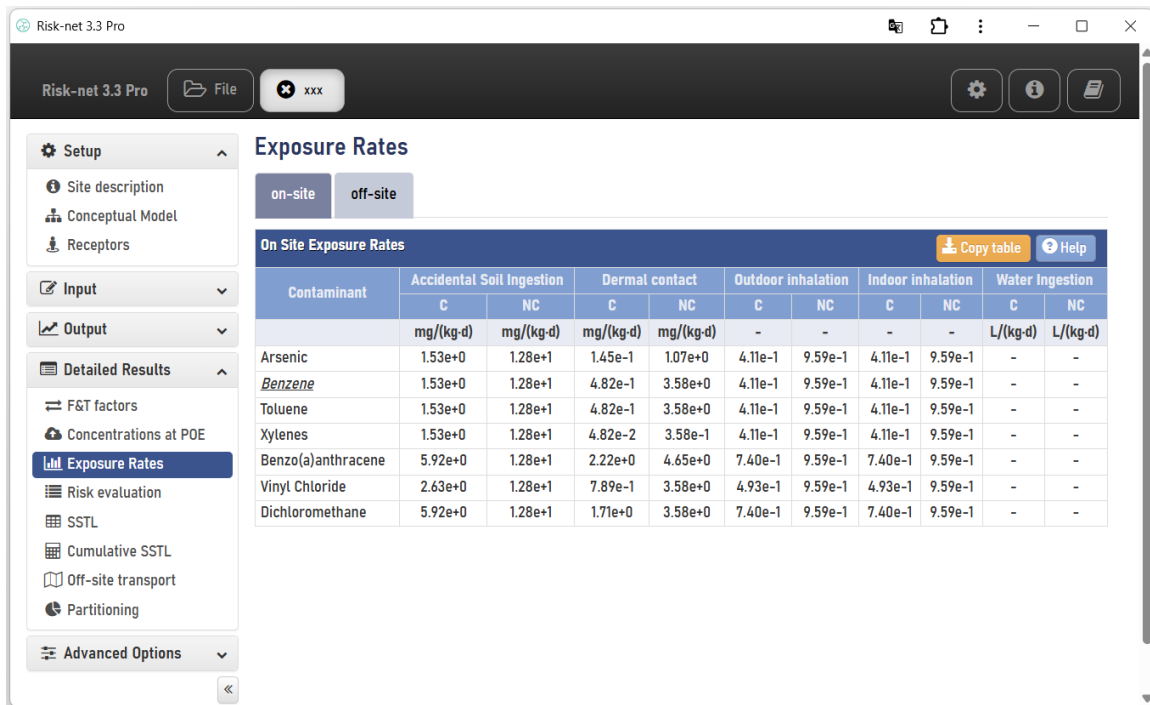


Figure 28. Exposure Rates.

DETAILED RISK EVALUATION

This screen displays the risks to human health, including individual risk (R) for each contaminant and cumulative risk (calculated as the sum of the risks for all selected contaminants), as well as the hazard index (HI) and the risk to groundwater resources (RGW), calculated for each source defined in the conceptual site model.

Risks exceeding acceptable limits are highlighted in red. Source concentrations exceeding the saturation concentration (or solubility, in the case of groundwater contamination) are highlighted in yellow.

On this screen, the user can iteratively determine the source concentration that ensures acceptable risk levels by entering a correction factor for each contaminant in the “f” column.

Contaminants for which physico-chemical and/or toxicological properties have been modified are displayed in italics and underlined.

Detailed results

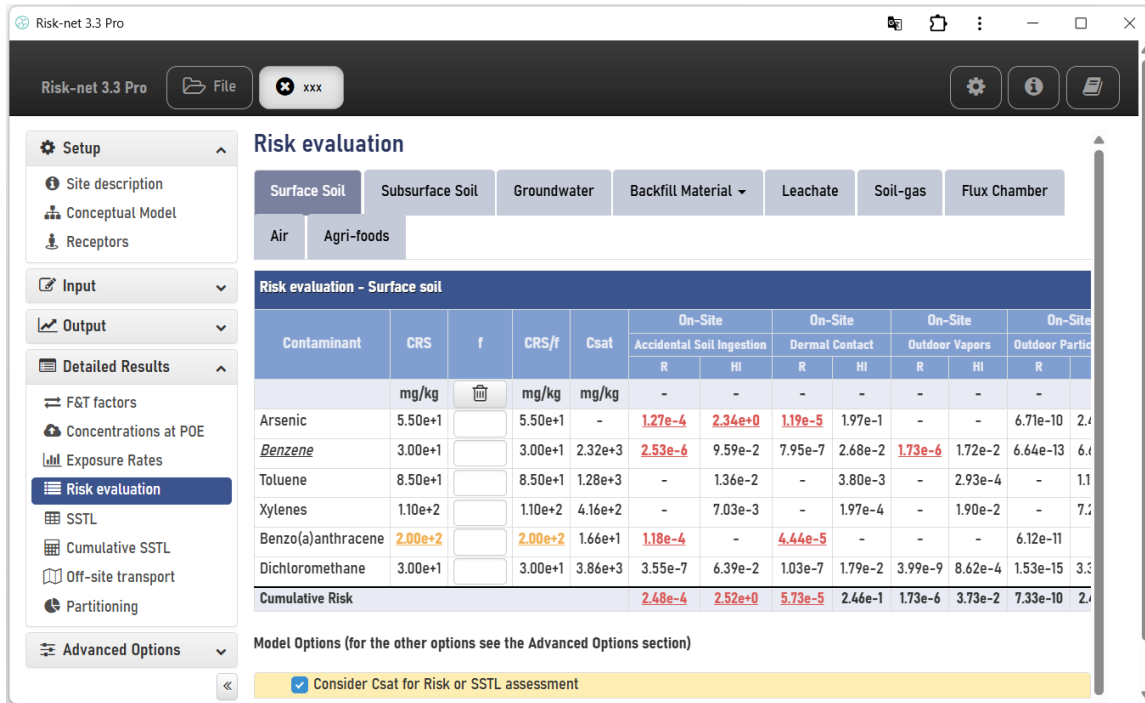


Figure 29. Detailed Risk Evaluation.

DETAILED SSTL EVALUATION

This screen displays the maximum acceptable concentrations in the affected source media (i.e., Site-Specific Target Levels, SSTLs) for each contaminant of concern, ensuring acceptable individual risks for human health (R and HI) and for groundwater resources (R_{gw}).

Contaminants for which the source concentration exceeds the calculated SSTL are highlighted in red. SSTLs that are lower than the PRG (Preliminary Remediation Goals) values defined in the database are marked with an asterisk.

Source concentrations exceeding the saturation concentration (or solubility, in the case of groundwater contamination) are highlighted in yellow.

Contaminants for which physico-chemical and/or toxicological properties have been modified are displayed in italics and underlined.

Detailed results

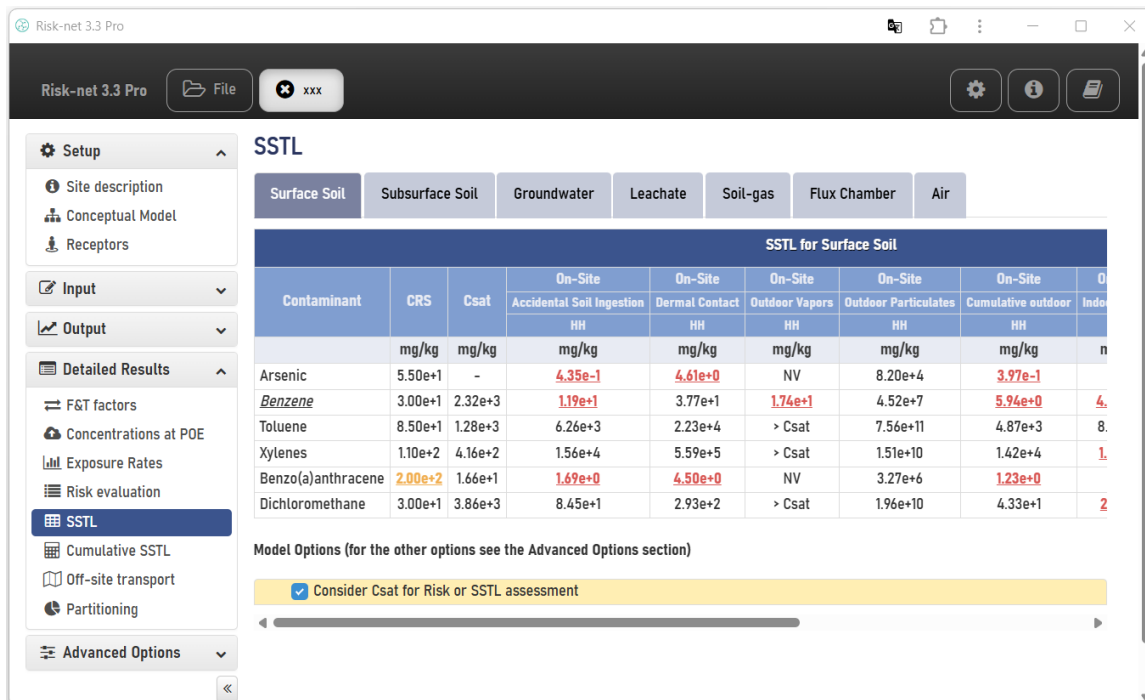


Figure 30. Detailed SSSL Evaluation.

OFF-SITE TRANSPORT

This screen allows the user to evaluate the off-site transport of contaminants in groundwater and in the atmosphere. The user must select the contaminant and the relevant matrix from the drop-down menu.

For groundwater transport, the graphs display the concentration of the selected contaminant as a function of both time and distance. For atmospheric dispersion, the graphs show concentration as a function of distance from the site.

The user can modify the distances and time intervals used in the calculations by editing the corresponding fields in the table.

At the bottom of the screen, a checkbox can be enabled to input the source's geographic coordinates. Based on these coordinates and the selected prevailing direction, the table displays the concentrations and reference coordinates of the calculated points.

In the groundwater dispersion model view, the following parameters are also provided for the selected contaminant: the retardation factor (R), the contaminant velocity in groundwater ($vc = ve / R$), the migration time to the point of compliance (POC) ($tc = x_{POC} / vc$), and the indicative time to reach steady-state conditions (tss), which is calculated iteratively by the software until the time-dependent concentration approaches the steady-state concentration.

Detailed results

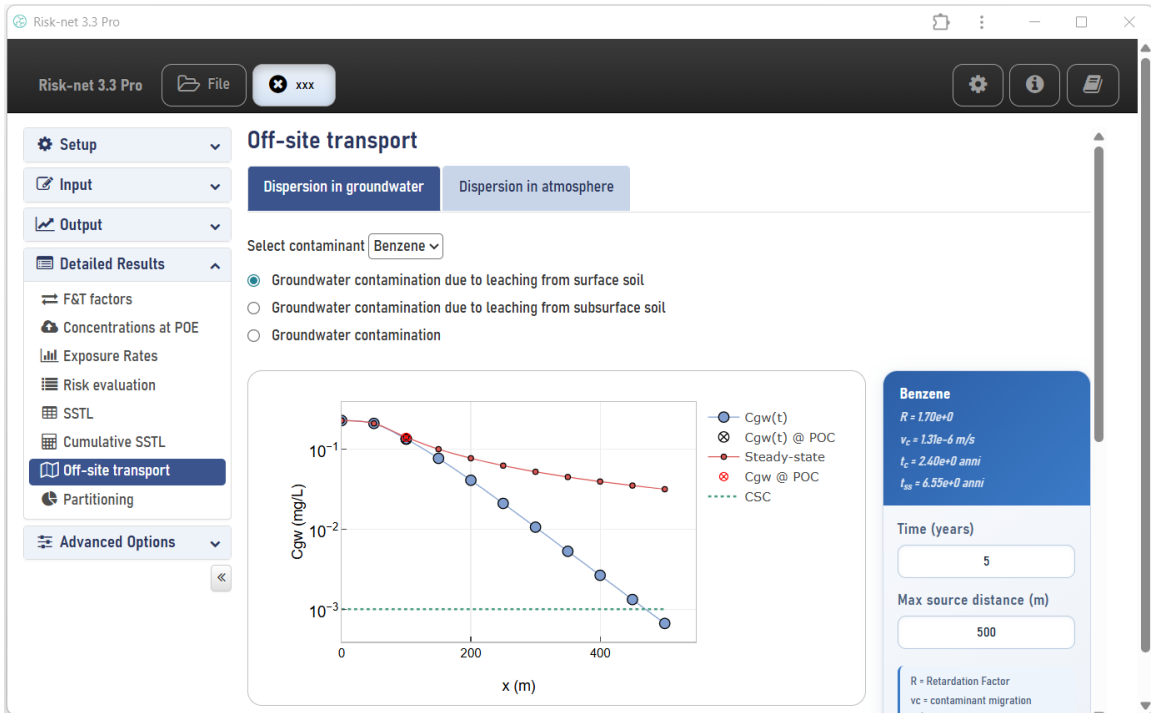


Figure 31. Off-site transport (groundwater).

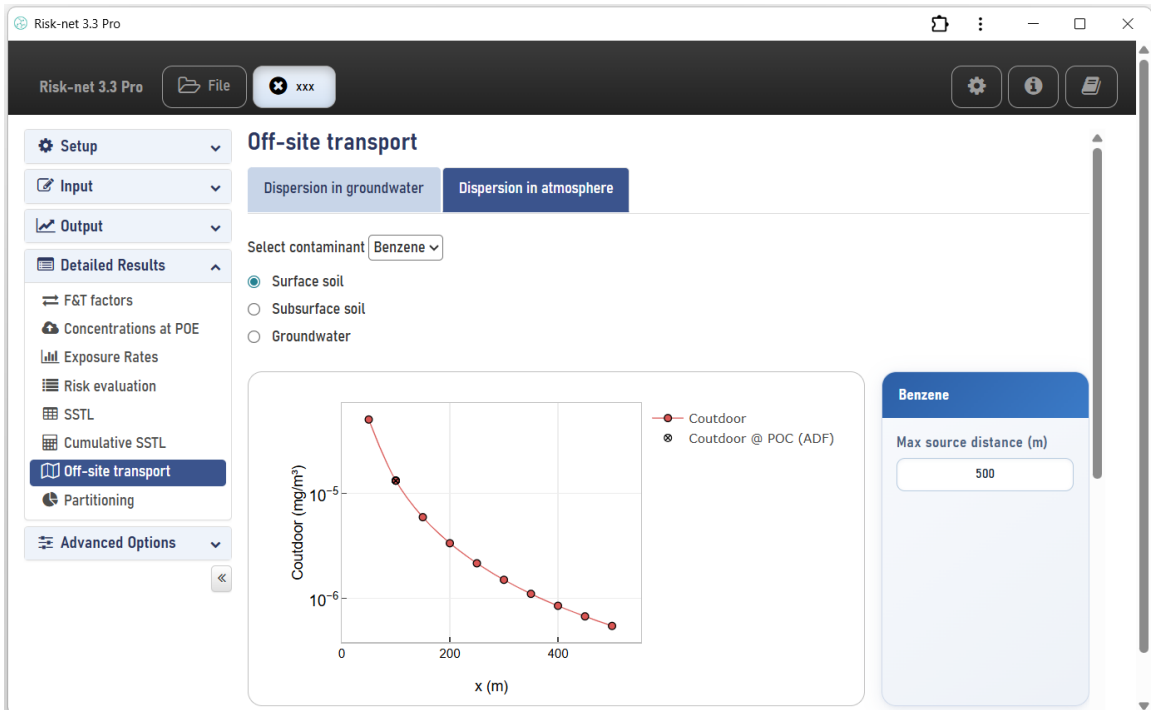


Figure 32. Off-site transport (atmosphere).

PARTITIONING

On this screen, the user must select the matrix (surface soil, subsurface soil, groundwater, or backfill material) and the contaminant of interest from the two drop-down menus. The contaminant must be selected among those previously defined as chemicals of concern.

Based on the selected matrix and contaminant, the screen displays the concentrations expected in different media (e.g., soil gas, eluate, outdoor air, indoor air), together with the corresponding measured values, if available.

This screen can be used to assess the reliability of the screening model in predicting the partitioning and transport of contaminants in the subsurface.

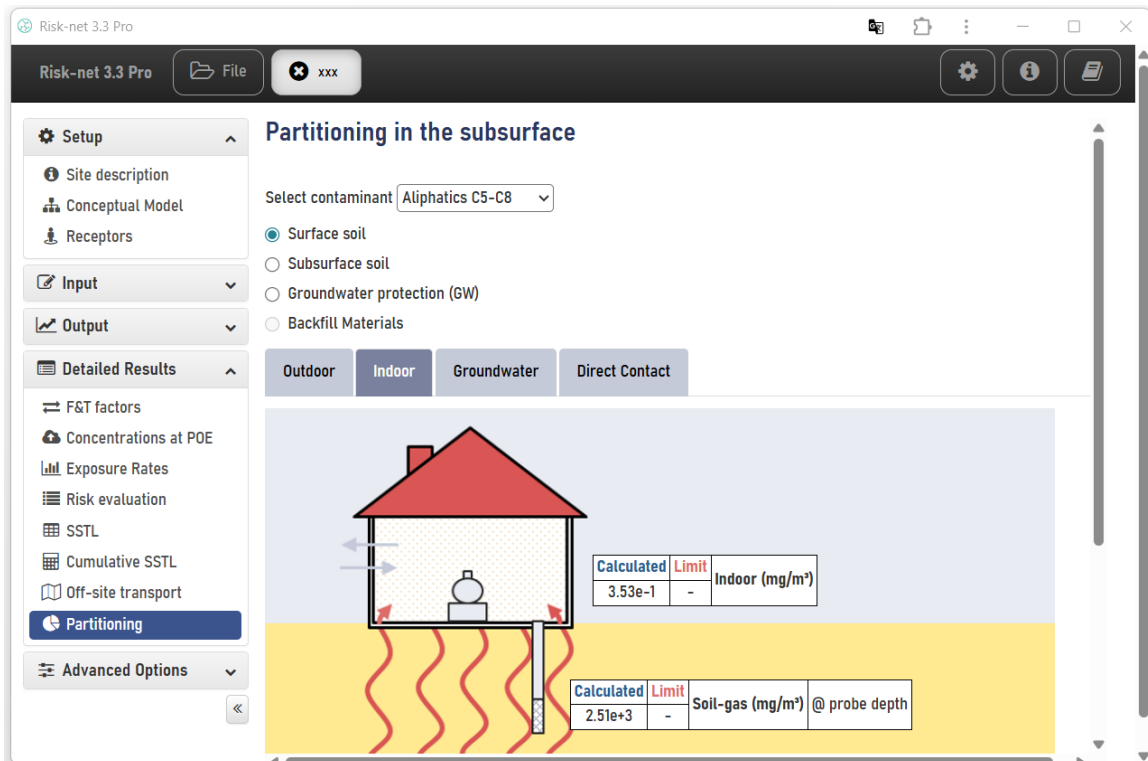


Figure 33. Concentrations Details.

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APPENDICES – EQUATIONS AND MODELING PROCEDURES

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

Individual Risk. The estimation of human health risk associated with exposure to a contaminant is performed in the software using the following equations:

$$R = E \cdot SF \quad \text{Risk for carcinogenic contaminants}$$

$$HI = E / RfD \quad \text{Hazard Index for non-carcinogenic contaminants}$$

where E is the chronic daily exposure rate, SF is the slope factor (i.e., the incremental probability of cancer per unit dose), and RfD is the reference dose (i.e., the daily exposure level that is not expected to cause adverse effects over a lifetime).

The chronic daily exposure, E , is calculated by multiplying the contaminant concentration at the point of exposure (C_{poe}) by the effective exposure rate (EM), such as the daily amount of soil ingested or the volume of air inhaled per unit body weight:

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

The concentration at the point of exposure (C_{poe}) is calculated as:

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

where CRS is the representative source concentration and FT is the fate and transport factor associated with the selected migration pathway.

By combining these equations, risk and hazard index values can be determined as follows:

$$R = FT \cdot CRS \cdot EM \cdot SF \quad \text{Risk for carcinogenic contaminants}$$

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

These calculations are performed for each active exposure and migration pathway at the site, using the appropriate exposure factors and fate and transport factors (see the tables below for details). The equations used to calculate the different fate and transport factors (FT) are provided in Appendix 3, while those for intake rates are reported in Appendix 4.

It should be noted that the equations presented above follow the ISPRA guidelines (2008), which are based on the use of Reference Dose (*RfD*) and Slope Factor (*SF*). However, for the inhalation pathway, the software also allows the use of an alternative approach based on Reference Concentration (*RfC*) and Inhalation Unit Risk (*IUR*), using the following equations:

$$R = FT \cdot CRS \cdot EC \cdot IUR \quad \text{Risk for carcinogenic contaminants}$$

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

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

Multiple exposure pathways. The following section describes the criteria adopted by the software for calculating individual risk for each medium of concern, taking into account multiple exposure pathways.

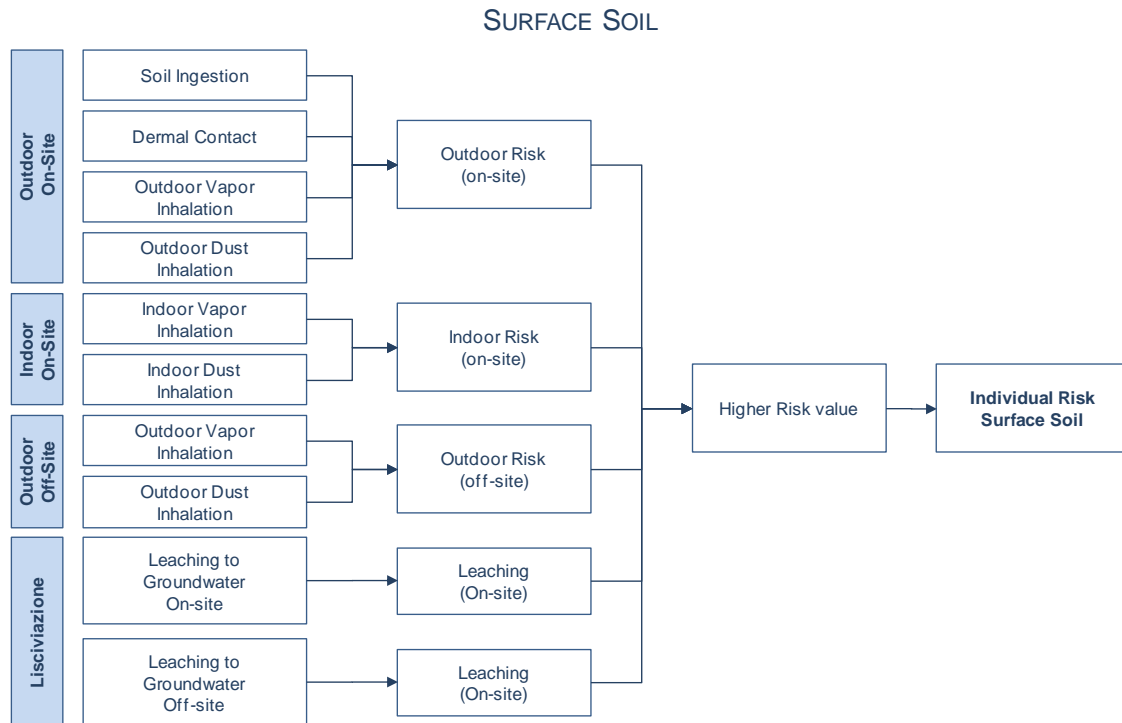


Figure 34. Risk – Surface soil. Multiple exposures.

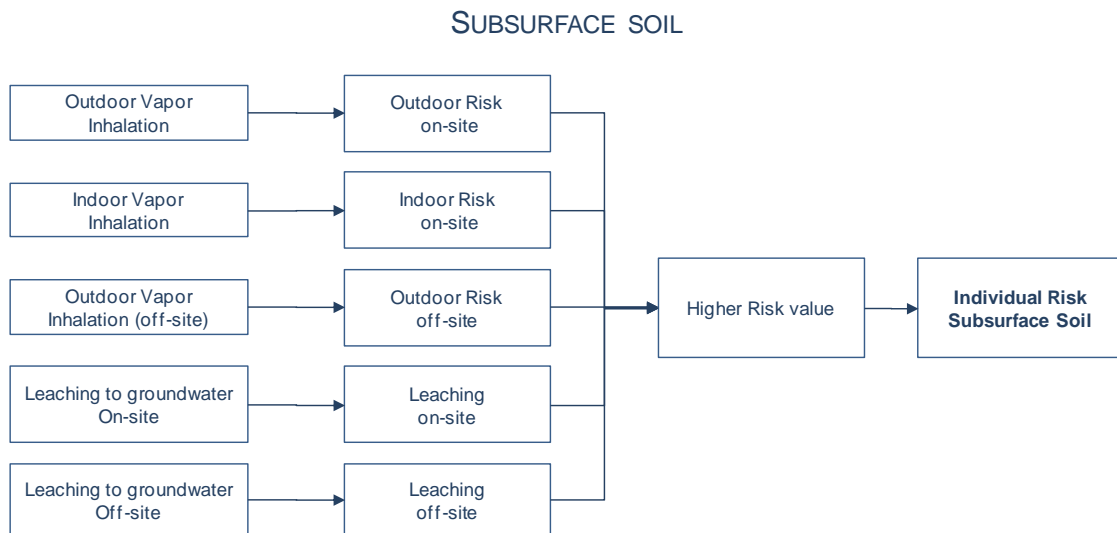


Figure 35. Risk – Subsurface soil. Multiple exposures.

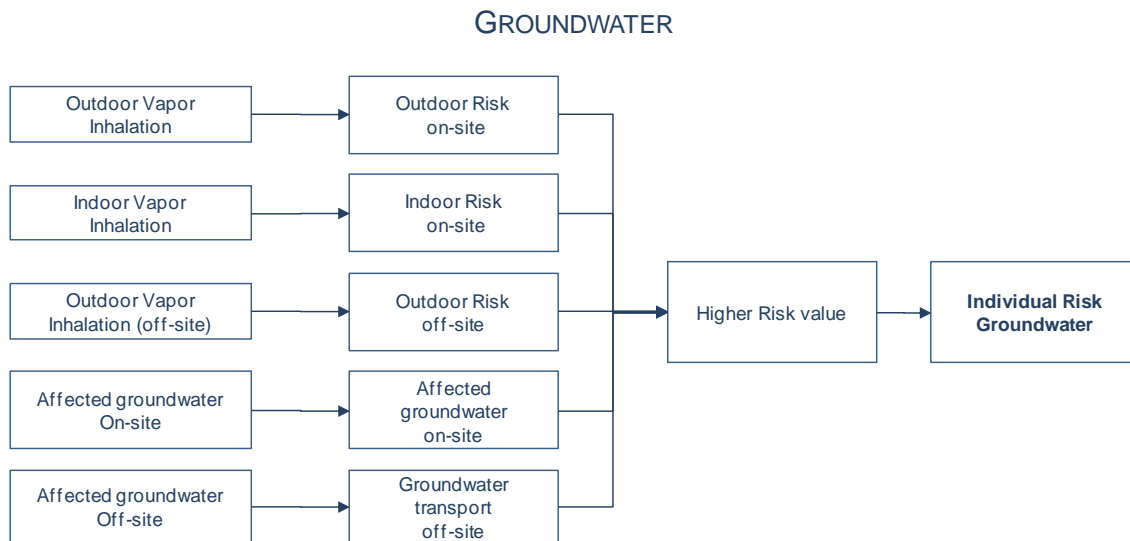


Figure 36. Risk – Groundwater. Multiple exposures.

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

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

Cumulative risk for carcinogenic contaminants

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

Risk for the groundwater resource. The risk to groundwater resources (R_{GW}) is evaluated by comparing the contaminant concentration in groundwater at the point of compliance (POC) with the reference values established for groundwater protection (e.g., Maximum Contaminant Levels, MCLs):

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

Table 9. Surface Soil: Risk and Hazard Index	
<p>Soil Ingestion (no off-site)</p> $R_{SS.IngS} = CRS \cdot SF_{Ing} \cdot EM_{IngS} \cdot 10^{-6} \text{ kg/mg}$ $HI_{SS.IngS} = CRS \cdot \frac{EM_{IngS} \cdot 10^{-6} \text{ kg/mg}}{RfD_{Ing}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SF_{Ing} = Slope factor - ingestion RfD_{Ing} = Reference dose - ingestion EM_{IngS} = Soil Ingestion rate</p>
<p>Dermal Contact (no off-site)</p> $R_{SS.ConD} = CRS \cdot SF_{Ing} \cdot EM_{ConD} \cdot 10^{-6} \text{ kg/mg}$ $HI_{SS.ConD} = CRS \cdot \frac{EM_{ConD} \cdot 10^{-6} \text{ kg/mg}}{RfD_{Ing}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SF_{Ing} = Slope factor for ingestion RfD_{Ing} = Reference dose - ingestion EM_{ConD} = Dermal contact rate</p>
<p>Outdoor Vapor Inhalation (reference dose method)</p> $R_{SS.InaO} = CRS \cdot SF_{Ina} \cdot EM_{InaO} \cdot VF_{ss} \cdot ADF$ $HI_{SS.InaO} = CRS \cdot \frac{EM_{InaO} \cdot VF_{ss} \cdot ADF}{RfD_{Ina}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose - inhalation EM_{InaO} = Outdoor inhalation rate VF_{ss} = Outdoor volatilization factor ADF = Atmospheric dispersion factor</p>
<p>Outdoor Vapor Inhalation (reference concentration method)</p> $R_{SS.InaO} = CRS \cdot IUR_{Ina} \cdot EC_{InaO} \cdot VF_{ss} \cdot ADF$ $HI_{SS.InaO} = CRS \cdot \frac{EC_{InaO} \cdot VF_{ss} \cdot ADF}{RfC_{Ina}}$	<p>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</p>
<p>Outdoor Dust Inhalation (reference dose method)</p> $R_{SS.InaOP} = CRS \cdot SF_{Ina} \cdot EM_{InaO} \cdot PEF \cdot ADF$ $HI_{SS.InaOP} = CRS \cdot \frac{EM_{InaO} \cdot PEF \cdot ADF}{RfD_{Ina}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose - inhalation EM_{InaO} = Outdoor inhalation rate PEF = Particulate emission factor ADF = Atmospheric dispersion factor</p>
<p>Outdoor Dust Inhalation (reference concentration method)</p> $R_{SS.InaOP} = CRS \cdot IUR \cdot EC_{InaO} \cdot PEF \cdot ADF$ $HI_{SS.InaOP} = CRS \cdot \frac{EC_{InaO} \cdot PEF \cdot ADF}{RfC}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration IUR_{Ina} = Inhalation Unit Risk RfC_{Ina} = Reference concentration EC_{InaO} = Outdoor inhalation rate PEF = Particulate emission factor ADF = Atmospheric dispersion factor</p>
<p>Outdoor cumulative risk</p> $R_{SS.outdoor} = R_{SS.IngS} + R_{SS.ConD} + R_{SS.InaO} + R_{SS.InaOP}$ $HI_{SS.outdoor} = HI_{SS.IngS} + HI_{SS.ConD} + HI_{SS.InaO} + HI_{SS.InaOP}$	

Table 9. Surface Soil: Risk and Hazard Index	
<p>Indoor Vapor Inhalation (no off-site) (reference dose method)</p> $R_{SS.Inal} = CRS \cdot SF_{Ina} \cdot EM_{Inal} \cdot VF_{ssesp}$ $HI_{SS.Inal} = CRS \cdot \frac{EM_{Inal} \cdot VF_{ssesp}}{RfD_{Ina}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI_{na} = Slope factor - inhalation RfD_{ina} = Reference dose - inhalation EM_{Inal} = Indoor inhalation rate VF_{ssesp} = Indoor volatilization factor</p>
<p>Indoor Vapor Inhalation (no off-site) (reference concentration method)</p> $R_{SS.Inal} = CRS \cdot IUR_{Ina} \cdot EC_{Inal} \cdot VF_{ssesp}$ $HI_{SS.Inal} = CRS \cdot \frac{EC_{Inal} \cdot VF_{ssesp}}{RfC_{Ina}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration IUR_{ina} = Inhalation Unit Risk RfC_{ina} = Reference concentration EC_{Inal} = Indoor inhalation rate VF_{ssesp} = Indoor volatilization factor</p>
<p>Indoor Dust Inhalation (no off-site) (reference dose method)</p> $R_{SS.InalP} = CRS \cdot SF_{Ina} \cdot EM_{Inal} \cdot PEF_{in}$ $HI_{SS.InalP} = CRS \cdot \frac{EM_{Inal} \cdot PEF_{in}}{RfD_{Ina}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI_{na} = Slope factor - inhalation RfD_{ina} = Reference dose - inhalation EM_{Inal} = Indoor inhalation rate PEF_{in} = Particulate indoor emission factor</p>
<p>Indoor Dust Inhalation (no off-site) (reference concentration method)</p> $R_{SS.InalP} = CRS \cdot IUR \cdot EC_{Inal} \cdot PEF_{in}$ $HI_{SS.InalP} = CRS \cdot \frac{EC_{Inal} \cdot PEF_{in}}{RfC}$	<p>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</p>
<p>Indoor cumulative risk</p> $R_{SS.Indoor} = R_{SS.Inal} + R_{SS.InalP}$ $HI_{SS.Indoor} = HI_{SS.Inal} + HI_{SS.InalP}$	
<p>Ingestion of water</p> $R_{SS.LF} = CRS \cdot \frac{SF_{Ing} \cdot EM_{IngW} \cdot LF_{ss}}{DAF}$ $HI_{SS.LF} = CRS \cdot \frac{EM_{IngW} \cdot LF_{ss}}{RfD_{Ing} \cdot DAF}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI_{ng} = Slope factor - ingestion RfD_{ing} = Reference dose - ingestion EM_{IngW} = Water Ingestion rate LF_{ss} = Leaching factor DAF = Groundwater dilution factor</p>
<p>Risk and Hazard Index for surface soil</p> $R_{SS} = \max [R_{SS.outdoor}; R_{SS.Indoor}; R_{SS.LF}]$ $HI_{SS} = \max [HI_{SS.outdoor}; HI_{SS.Indoor}; HI_{SS.LF}]$	

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

Table 10. Subsurface Soil: Risk and Hazard Index	
<p>Outdoor Vapor Inhalation (reference dose method)</p> $R_{SP.InaO} = CRS \cdot SF_{Ina} \cdot VF_{samb} \cdot EM_{InaO} \cdot ADF$ $HI_{SP.InaO} = CRS \cdot \frac{VF_{samb} \cdot EM_{InaO} \cdot ADF}{RfD_{Ina}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI_{na} = Slope factor - inhalation RfD_{Ina} = Reference dose - inhalation EM_{InaO} = Outdoor inhalation rate VF_{samb} = Outdoor volatilization factor ADF = Atmospheric dispersion factor</p>
<p>Outdoor Vapor Inhalation (reference concentration method)</p> $R_{SP.InaO} = CRS \cdot IUR_{Ina} \cdot VF_{samb} \cdot EC_{InaO} \cdot ADF$ $HI_{SP.InaO} = CRS \cdot \frac{VF_{samb} \cdot EC_{InaO} \cdot ADF}{RfC_{Ina}}$	<p>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</p>
<p>Indoor Vapor Inhalation (no off-site) (reference dose method)</p> $R_{SP.Inal} = CRS \cdot SF_{Ina} \cdot VF_{seps} \cdot EM_{Inal}$ $HI_{SP.Inal} = CRS \cdot \frac{VF_{seps} \cdot EM_{Inal}}{RfD_{Ina}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI_{na} = Slope factor - inhalation RfD_{Ina} = Reference dose - inhalation EM_{Inal} = Indoor inhalation rate VF_{seps} = Indoor volatilization factor</p>
<p>Indoor Vapor Inhalation (no off-site) (reference concentration method)</p> $R_{SP.Inal} = CRS \cdot IUR_{Ina} \cdot VF_{seps} \cdot EC_{Inal}$ $HI_{SP.Inal} = CRS \cdot \frac{VF_{seps} \cdot EC_{Inal}}{RfC_{Ina}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration IUR_{Ina} = Inhalation Unit Risk RfC_{Ina} = Reference concentration EC_{Inal} = Indoor inhalation rate VF_{seps} = Indoor volatilization factor</p>
<p>Ingestion of water</p> $R_{SP.LF} = CRS \cdot \frac{SF_{Ing} \cdot EM_{IngW} \cdot LF_{sp}}{DAF}$ $HI_{SP.LF} = CRS \cdot \frac{EM_{IngW} \cdot LF_{sp}}{RfD_{Ing} \cdot DAF}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI_{ng} = Slope factor - ingestion RfD_{Ing} = Reference dose - ingestion EM_{IngW} = Water Ingestion rate LF_{sp} = Leaching factor DAF = Groundwater dilution factor</p>
<p>Risk and Hazard Index for subsurface soil</p> $R_{SP} = \max [R_{SP.InaO}; R_{SP.Inal}; R_{SP.LF}]$ $HI_{SP} = \max [HI_{SP.InaO}; HI_{SP.Inal}; HI_{SP.LF}]$	

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

Table 11. Groundwater: Risk and Hazard Index	
<p>Outdoor Vapor Inhalation (reference dose method)</p> $R_{GW.InaO} = CRS \cdot \frac{SF_{Ina} \cdot VF_{wamb} \cdot EM_{InaO}}{DAF}$ $HI_{GW.InaO} = CRS \cdot \frac{VF_{wamb} \cdot EM_{InaO}}{RfD_{Ina} \cdot DAF}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI_{na} = Slope factor - inhalation RfD_{ina} = Reference dose - inhalation EM_{inaO} = Outdoor inhalation rate VF_{wamb} = Outdoor volatilization factor DAF = Groundwater dilution factor</p>
<p>Outdoor Vapor Inhalation (reference concentration method)</p> $R_{GW.InaO} = CRS \cdot \frac{IUR_{Ina} \cdot VF_{wamb} \cdot EC_{InaO}}{DAF}$ $HI_{GW.InaO} = CRS \cdot \frac{VF_{wamb} \cdot EC_{InaO}}{RfC_{Ina} \cdot DAF}$	<p>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</p>
<p>Indoor Vapor Inhalation (reference dose method)</p> $R_{GW.Inal} = CRS \cdot \frac{SF_{Ina} \cdot VF_{wesp} \cdot EM_{Inal}}{DAF}$ $HI_{GW.Inal} = CRS \cdot \frac{VF_{wesp} \cdot EM_{Inal}}{RfD_{Ina} \cdot DAF}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI_{na} = Slope factor - inhalation RfD_{ina} = Reference dose - inhalation EM_{inal} = Indoor inhalation rate VF_{wesp} = Indoor volatilization factor DAF = Groundwater dilution factor</p>
<p>Indoor Vapor Inhalation (reference concentration method)</p> $R_{GW.Inal} = CRS \cdot \frac{IUR_{Ina} \cdot VF_{wesp} \cdot EC_{Inal}}{DAF}$ $HI_{GW.Inal} = CRS \cdot \frac{VF_{wesp} \cdot EC_{Inal}}{RfC_{Ina} \cdot DAF}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration IUR_{ina} = Inhalation Unit Risk RfC_{ina} = Reference concentration EC_{inal} = Indoor inhalation rate VF_{wesp} = Indoor volatilization factor DAF = Groundwater dilution factor</p>
<p>Ingestion of water</p> $R_{GW.D} = CRS \cdot \frac{SF_{Ing} \cdot EM_{IngW}}{DAF}$ $HI_{GW.D} = CRS \cdot \frac{EM_{IngW}}{RfD_{Ing} \cdot DAF}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SFI_{ng} = Slope factor - ingestion RfD_{ing} = Reference dose - ingestion EM_{ingW} = Water Ingestion rate DAF = Groundwater dilution factor</p>
<p>Risk and Hazard Index for groundwater</p> $R_{GW} = \max [R_{GW.InaO}; R_{GW.Inal}; R_{GW.D}]$ $HI_{GW} = \max [HI_{GW.InaO}; HI_{GW.Inal}; HI_{GW.D}]$	

For On-site Receptors DAF = 1

Table 12. Risk for the groundwater resource	
<p>Surface Soil – Leaching to Groundwater</p> $R_{SS.LF} = \frac{CRS \cdot LF_{ss}}{DAF \cdot MCL_{GW}}$	<p>CRS = Source Concentration MCL_{GW} = Maximum Contaminant Level LF_{ss} = Leaching factor DAF = Groundwater dilution factor</p>
<p>Subsurface Soil – Leaching to Groundwater</p> $R_{SP.LF} = \frac{CRS \cdot LF_{sp}}{DAF \cdot MCL_{GW}}$	<p>CRS = Source Concentration MCL_{GW} = Maximum Contaminant Level LF_{sp} = Leaching factor DAF = Groundwater dilution factor</p>
<p>Affected groundwater</p> $R_{GW.D} = \frac{CRS}{DAF \cdot MCL_{GW}}$	<p>CRS = Source Concentration MCL_{GW} = Maximum Contaminant Level DAF = Groundwater dilution factor</p>

For On-site Receptors DAF = 1

APP. 1B. RISK CALCULATION (BACKFILL MATERIALS)

Table 13. Backfill Materials: Risk and Hazard Index	
<p>Soil ingestion (no off-site)</p> $R_{\text{MdR.IngS}} = \text{CRS}_{\text{ss}} \cdot \text{SF}_{\text{Ing}} \cdot \text{EM}_{\text{IngS}} \cdot 10^{-6} \text{ kg/mg}$ $\text{HI}_{\text{MdR.IngS}} = \text{CRS}_{\text{ss}} \cdot \frac{\text{EM}_{\text{IngS}} \cdot 10^{-6} \text{ kg/mg}}{\text{RfD}_{\text{Ing}}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SF_{Ing} = Slope factor - ingestion RfD_{Ing} = Reference dose - ingestion EM_{IngS} = Soil Ingestion rate</p>
<p>Dermal Contact (no off-site)</p> $R_{\text{MdR.ConD}} = \text{CRS}_{\text{ss}} \cdot \text{SF}_{\text{Ing}} \cdot \text{EM}_{\text{ConD}} \cdot 10^{-6} \text{ kg/mg}$ $\text{HI}_{\text{MdR.ConD}} = \text{CRS}_{\text{ss}} \cdot \frac{\text{EM}_{\text{ConD}} \cdot 10^{-6} \text{ kg/mg}}{\text{RfD}_{\text{Ing}}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SF_{Ing} = Slope factor for ingestion RfD_{Ing} = Reference dose - ingestion EM_{ConD} = Dermal contact rate</p>
<p>Outdoor Vapor Inhalation (reference dose method)</p> $R_{\text{MdR.InaO}} = \text{CRS}_{\text{tot}} \cdot \text{SF}_{\text{Ina}} \cdot \text{EM}_{\text{InaO}} \cdot \text{VF}_{\text{MdR}} \cdot \text{ADF}$ $\text{HI}_{\text{MdR.InaO}} = \text{CRS}_{\text{tot}} \cdot \frac{\text{EM}_{\text{InaO}} \cdot \text{VF}_{\text{MdR}} \cdot \text{ADF}}{\text{RfD}_{\text{Ina}}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose - inhalation EM_{InaO} = Outdoor inhalation rate VF_{MdR} = Outdoor volatilization factor ADF = Atmospheric dispersion factor</p>
<p>Outdoor Vapor Inhalation (reference concentration method)</p> $R_{\text{MdR.InaO}} = \text{CRS}_{\text{tot}} \cdot \text{IUR} \cdot \text{EC}_{\text{InaO}} \cdot \text{VF}_{\text{MdR}} \cdot \text{ADF}$ $\text{HI}_{\text{MdR.InaO}} = \text{CRS}_{\text{tot}} \cdot \frac{\text{EC}_{\text{InaO}} \cdot \text{VF}_{\text{MdR}} \cdot \text{ADF}}{\text{RfC}}$	<p>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</p>
<p>Outdoor Dust Inhalation (reference dose method)</p> $R_{\text{MdR.InaOP}} = \text{CRS}_{\text{ss}} \cdot \text{SF}_{\text{Ina}} \cdot \text{EM}_{\text{InaO}} \cdot \text{PEF} \cdot \text{ADF}$ $\text{HI}_{\text{MdR.InaOP}} = \text{CRS}_{\text{ss}} \cdot \frac{\text{EM}_{\text{InaO}} \cdot \text{PEF} \cdot \text{ADF}}{\text{RfD}_{\text{Ina}}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose - inhalation EM_{InaO} = Outdoor inhalation rate PEF = Particulate emission factor ADF = Atmospheric dispersion factor</p>
<p>Outdoor Dust Inhalation (reference concentration method)</p> $R_{\text{MdR.InaOP}} = \text{CRS}_{\text{ss}} \cdot \text{IUR} \cdot \text{EC}_{\text{InaO}} \cdot \text{PEF} \cdot \text{ADF}$ $\text{HI}_{\text{MdR.InaOP}} = \text{CRS}_{\text{ss}} \cdot \frac{\text{EC}_{\text{InaO}} \cdot \text{PEF} \cdot \text{ADF}}{\text{RfC}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration IUR_{Ina} = Inhalation Unit Risk RfC_{Ina} = Reference concentration EC_{InaO} = Outdoor inhalation rate PEF = Particulate emission factor ADF = Atmospheric dispersion factor</p>

Table 13. Backfill Materials: Risk and Hazard Index	
Outdoor cumulative risk	
$R_{Mdr.outdoor} = R_{Mdr.IngS} + R_{Mdr.ConD} + R_{Mdr.InaO} + R_{Mdr.InaOP}$ $HI_{Mdr.outdoor} = HI_{Mdr.IngS} + HI_{Mdr.ConD} + HI_{Mdr.InaO} + HI_{Mdr.InaOP}$	
Indoor Vapor Inhalation (no off-site) (reference dose method) $R_{Mdr.Inal} = CRS_{tot} \cdot SF_{Ina} \cdot EM_{Inal} \cdot VF_{Mdr,esp}$ $HI_{Mdr.Inal} = CRS_{tot} \cdot \frac{EM_{Inal} \cdot VF_{Mdr,esp}}{RfD_{Ina}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SF _{Ina} = Slope factor - inhalation RfD _{Ina} = Reference dose - inhalation EM _{Inal} = Indoor inhalation rate VF _{MdResp} = Indoor volatilization factor
Indoor Vapor Inhalation (no off-site) (reference concentration method) $R_{Mdr.Inal} = CRS_{tot} \cdot IUR \cdot EC_{Inal} \cdot VF_{Mdr,esp}$ $HI_{Mdr.Inal} = CRS_{tot} \cdot \frac{EC_{Inal} \cdot VF_{Mdr,esp}}{RfC}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration IUR _{Ina} = Inhalation Unit Risk RfC _{Ina} = Reference concentration EC _{Inal} = Indoor inhalation rate VF _{MdResp} = Indoor volatilization factor
Indoor Dust Inhalation (no off-site) (reference dose method) $R_{Mdr.InalP} = CRS_{ss} \cdot SF_{Ina} \cdot EM_{Inal} \cdot PEF_{in}$ $HI_{Mdr.InalP} = CRS_{ss} \cdot \frac{EM_{Inal} \cdot PEF_{in}}{RfD_{Ina}}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SF _{Ina} = Slope factor - inhalation RfD _{Ina} = Reference dose - inhalation EM _{Inal} = Indoor inhalation rate PEF _{in} = Particulate indoor emission factor
Indoor Dust Inhalation (no off-site) (reference concentration method) $R_{Mdr.InalP} = CRS_{ss} \cdot IUR \cdot EC_{Inal} \cdot PEF_{in}$ $HI_{Mdr.InalP} = CRS_{ss} \cdot \frac{EC_{Inal} \cdot PEF_{in}}{RfC}$	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	
$R_{Mdr.Indoor} = R_{Mdr.Inal} + R_{Mdr.InalP}$ $HI_{Mdr.Indoor} = HI_{Mdr.Inal} + HI_{Mdr.InalP}$	
Ingestion of water $R_{Mdr.LF} = CRS_{tot} \cdot \frac{SF_{Ing} \cdot EM_{IngW} \cdot LF_{Mdr}}{DAF}$ $HI_{Mdr.LF} = CRS_{tot} \cdot \frac{EM_{IngW} \cdot LF_{Mdr}}{RfD_{Ing} \cdot DAF}$	R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SF _{Ing} = Slope factor - ingestion RfD _{Ing} = Reference dose - ingestion EM _{IngW} = Water Ingestion rate LF _{MdR} = Leaching factor DAF = Groundwater dilution
Risk and Hazard Index for Backfill Materials $R_{Mdr} = \max [R_{Mdr.outdoor}; R_{Mdr.Indoor}; R_{Mdr.LF}]$ $HI_{Mdr} = \max [HI_{Mdr.outdoor}; HI_{Mdr.Indoor}; HI_{Mdr.LF}]$	

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

Table 14. Backfill Material: risk for the groundwater resource

<p>Leaching from Backfill Material</p> $R_{Mdr.LF} = \frac{CRS_{tot} \cdot LF_{Mdr}}{DAF \cdot MCL_{GW} \cdot 10^{-3} \text{ mg}/\mu\text{g}}$	<p>CRS = Source Concentration MCL_{GW} = Maximum Contaminant Level L_{sMdr} = Leaching factor DAF = Groundwater dilution factor</p>
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For On-site Receptors DAF = 1

Table 15. Eluate Backfill Material: Risk and Hazard Index

<p>Water Ingestion</p> $R_{EL,Mdr.D} = CRS \cdot \frac{\alpha_{LF,Mdr} \cdot SF_{Ing} \cdot EM_{IngW}}{DAF}$ $HI_{EL,Md.D} = CRS \cdot \frac{\alpha_{LF,Mdr} \cdot EM_{IngW}}{RfD_{Ing} \cdot DAF}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Source Concentration SF_{Ing} = Slope factor - ingestion RfD_{Ing} = Reference dose - ingestion EM_{IngW} = Water Ingestion rate α_{LF,Mdr} = Leaching factor DAF = Groundwater dilution factor</p>
<p>Leaching from Backfill Material</p> $R_{GW.EL,Mdr} = \frac{CRS \cdot \alpha_{LF,Mdr}}{DAF \cdot MCL_{GW} \cdot 10^{-3} \text{ mg}/\mu\text{g}}$	<p>CRS = Source Concentration MCL_{GW} = Maximum Contaminant Level α_{LF,Mdr} = Leaching factor DAF = Groundwater dilution factor</p>

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

Table 16. Soil-gas: Risk and Hazard Index	
<p>Outdoor Vapor Inhalation (reference dose method)</p> $R_{SG.InaO} = CRS \cdot SF_{Ina} \cdot \alpha_{samb} \cdot EM_{InaO} \cdot ADF$ $HI_{SG.InaO} = CRS \cdot \frac{\alpha_{samb} \cdot EM_{InaO} \cdot ADF}{RfD_{Ina}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Representative Concentration SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose - inhalation EM_{InaO} = Outdoor inhalation rate α_{samb} = Outdoor volatilization factor ADF = Atmospheric dispersion factor</p>
<p>Outdoor Vapor Inhalation (reference concentration method)</p> $R_{SG.InaO} = CRS \cdot IUR \cdot \alpha_{samb} \cdot EC_{InaO} \cdot ADF$ $HI_{SG.InaO} = CRS \cdot \frac{\alpha_{samb} \cdot EC_{InaO} \cdot ADF}{RfC}$	<p>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</p>
<p>Indoor Vapor Inhalation (reference dose method)</p> $R_{SG.Inal} = CRS \cdot SF_{Ina} \cdot \alpha_{seps} \cdot EM_{Inal}$ $HI_{SG.Inal} = CRS \cdot \frac{\alpha_{seps} \cdot EM_{Inal}}{RfD_{Ina}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Representative Concentration SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose - inhalation EM_{Inal} = Indoor inhalation rate α_{samb} = Indoor volatilization factor</p>
<p>Indoor Vapor Inhalation (reference concentration method)</p> $R_{SG.Inal} = CRS \cdot IUR \cdot \alpha_{seps} \cdot EC_{Inal}$ $HI_{SG.Inal} = CRS \cdot \frac{\alpha_{seps} \cdot EC_{Inal}}{RfC}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Representative Concentration IUR_{Ina} = Inhalation Unit Risk RfC_{Ina} = Reference concentration EC_{Inal} = Indoor inhalation rate α_{samb} = Indoor volatilization factor</p>

For On-site Receptors ADF = 1

Table 17. Flux-Chambers: Risk and Hazard Index	
<p>Outdoor Vapor Inhalation - Concentration (reference dose method)</p> $R_{FC.InaO} = CRS \cdot SF_{Ina} \cdot \alpha_{FC} \cdot EM_{InaO} \cdot ADF$ $HI_{FC.InaO} = CRS \cdot \frac{\alpha_{FC} \cdot EM_{InaO} \cdot ADF}{RfD_{Ina}}$	<p>R = Carcinogenic Risk HI = Hazard Index CRS = Representative Concentration SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose - inhalation EM_{InaO} = Outdoor inhalation rate α_{FC} = Outdoor volatilization factor ADF = Atmospheric dispersion factor</p>
<p>Outdoor Vapor Inhalation - Flux (reference concentration method)</p> $R_{FC.InaO} = CRS \cdot IUR \cdot \alpha_{FC} \cdot EC_{InaO} \cdot ADF$ $HI_{FC.InaO} = CRS \cdot \frac{\alpha_{FC} \cdot EC_{InaO} \cdot ADF}{RfC}$	<p>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</p>
<p>Outdoor Vapor Inhalation - Concentration (reference dose method)</p> $R_{FC.InaO} = F \cdot SF_{Ina} \cdot \alpha_{FC(flux)} \cdot EM_{InaO} \cdot ADF$ $HI_{FC.InaO} = F \cdot \frac{\alpha_{FC(flux)} \cdot EM_{InaO} \cdot ADF}{RfD_{Ina}}$	<p>R = Carcinogenic Risk HI = Hazard Index F = Measured Flux SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose - inhalation EM_{InaO} = Outdoor inhalation rate α_{FC(flux)} = Outdoor volatilization factor ADF = Atmospheric dispersion factor</p>
<p>Outdoor Vapor Inhalation - Flux (reference concentration method)</p> $R_{FC.InaO} = F \cdot IUR \cdot \alpha_{FC(flux)} \cdot EC_{InaO} \cdot ADF$ $HI_{FC.InaO} = F \cdot \frac{\alpha_{FC(flux)} \cdot EC_{InaO} \cdot ADF}{RfC}$	<p>R = Carcinogenic Risk HI = Hazard Index F = Measured Flux IUR_{Ina} = Inhalation Unit Risk RfC_{Ina} = Reference concentration EC_{InaO} = Outdoor inhalation rate α_{FC(flux)} = Outdoor volatilization factor ADF = Atmospheric dispersion factor</p>

For On-site Receptors ADF = 1

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

For On-site Receptors ADF = 1

Table 19. Eluate (Surface Soil): Risk and Hazard Index	
<p>Water Ingestion</p> $R_{ELSS.D} = CRS \cdot \frac{\alpha_{LFSS} \cdot SF_{Ing} \cdot EM_{IngW}}{DAF}$ $HI_{ELSS.D} = CRS \cdot \frac{\alpha_{LFSS} \cdot EM_{IngW}}{RfD_{Ing} \cdot DAF}$	<p>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</p>
<p>Groundwater Protection</p> $R_{GW.ELSS} = \frac{CRS \cdot \alpha_{LFSS}}{DAF \cdot MCL_{GW}}$	<p>CRS = Representative Concentration MCL_{GW} = Maximum contaminant level α_{LFSS} = Leaching Factor DAF = Dilution Attenuation Factor</p>

For On-site Receptors $DAF=1$

Table 20. Eluate (Subsurface Soil): Risk and Hazard Index	
<p>Water Ingestion</p> $R_{ELsp.D} = CRS \cdot \frac{\alpha_{LFsp} \cdot SF_{Ing} \cdot EM_{IngW}}{DAF}$ $HI_{ELsp.D} = CRS \cdot \frac{\alpha_{LFsp} \cdot EM_{IngW}}{RfD_{Ing} \cdot DAF}$	<p>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</p>
<p>Groundwater Protection</p> $R_{GW.ELsp} = \frac{CRS \cdot \alpha_{LFsp}}{DAF \cdot MCL_{GW}}$	<p>CRS = Representative Concentration MCL_{GW} = Maximum contaminant level α_{LFsp} = Leaching Factor DAF = Dilution Attenuation Factor</p>

For On-site Receptors $DAF=1$

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

Table 21. Risk calculation for agri-food consumption	
<p>Average e Lifetime Average Daily Dose (ADD e LADD)</p> $ADD = [\sum_i (C \times IR)_i \times EF \times ED] / (BW \times AT_{ADD} \times 365)$ $LADD = [\sum_i (C \times IR)_i \times EF \times ED] / (BW \times AT_{LADD} \times 365)$ <p><i>This calculation is performed for each receptor (child, teenager, adult and senior)</i></p>	<p>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</p>
<p>Risk and Hazard Index</p> $HI = ADD/RfD$ $R = LADD \times SF$ <p><i>This calculation is performed for each receptor (child, teenager, adult and senior)</i></p>	<p>R = Carcinogenic Risk HI = Hazard Index ADD = Average Daily Dose LADD = Lifetime Average Daily Dose RfD = Reference Dose Ingestion SF = Slope Factor Ingestion</p>

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

The calculation of remediation targets (Individual Site-Specific Target Levels, *SSTLs*) is performed by applying the risk assessment procedure in backward mode. The resulting clean-up levels represent the maximum acceptable concentrations in the affected source media (soil or groundwater) that are protective of human health or groundwater receptors at the relevant points of exposure.

Individual Clean-up Levels (SSTL). Clean-up levels (*SSTLs*) are calculated using the same equations applied for risk estimation, rearranged and expressed in terms of source concentration:

$$SSTL = \frac{C_{poe}}{FT} = \frac{E}{EM \cdot FT} = \frac{TR}{SF \cdot EM \cdot FT} \quad \text{carcinogenic contaminants}$$

$$SSTL = \frac{C_{poe}}{FT} = \frac{E}{EM \cdot FT} = \frac{THI \cdot RfD}{EM \cdot FT} \quad \text{non-carcinogenic contaminants}$$

Where:

TR: Target Risk for a single contaminant (e.g. $TR = 10^{-6}$)

THI: Target Hazard Index for a single contaminant ($THI = 1$)

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 each active exposure and migration pathway at the site, using the appropriate exposure and fate and transport factors (see the tables below for details). The equations for the different fate and transport factors and intake rates are reported in the following sections.

It should be noted that the above equations are those reported in the ISPRA guidelines (2008), which are based on the use of Reference Dose (*RfD*) and Slope Factor (*SF*). However, for the inhalation pathway, the software also allows the use of an alternative approach based on Reference Concentration (*RfC*) and Inhalation Unit Risk (*IUR*), using the following equations:

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

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

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

Multiple exposure pathways. The equations described above provide the *SSTL* for a single exposure pathway. The Individual *SSTL* (associated with a single contaminant) is derived by accounting for the combined effects of multiple exposure pathways.

This is achieved by first calculating the *SSTLs* for each exposure scenario (e.g., outdoor exposure) and then selecting the most conservative value (i.e., the lowest *SSTL*). The combined effect of multiple exposure pathways is evaluated as the reciprocal of the sum of the reciprocals of the *SSTLs* calculated for each exposure route.

For example, in the case of outdoor exposure, the combined *SSTL* can be expressed as:

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

For other exposure scenarios, refer to the tables below.

The following figures illustrate the criteria adopted by the software for calculating individual clean-up levels for each medium of concern, taking into account multiple exposure pathways.

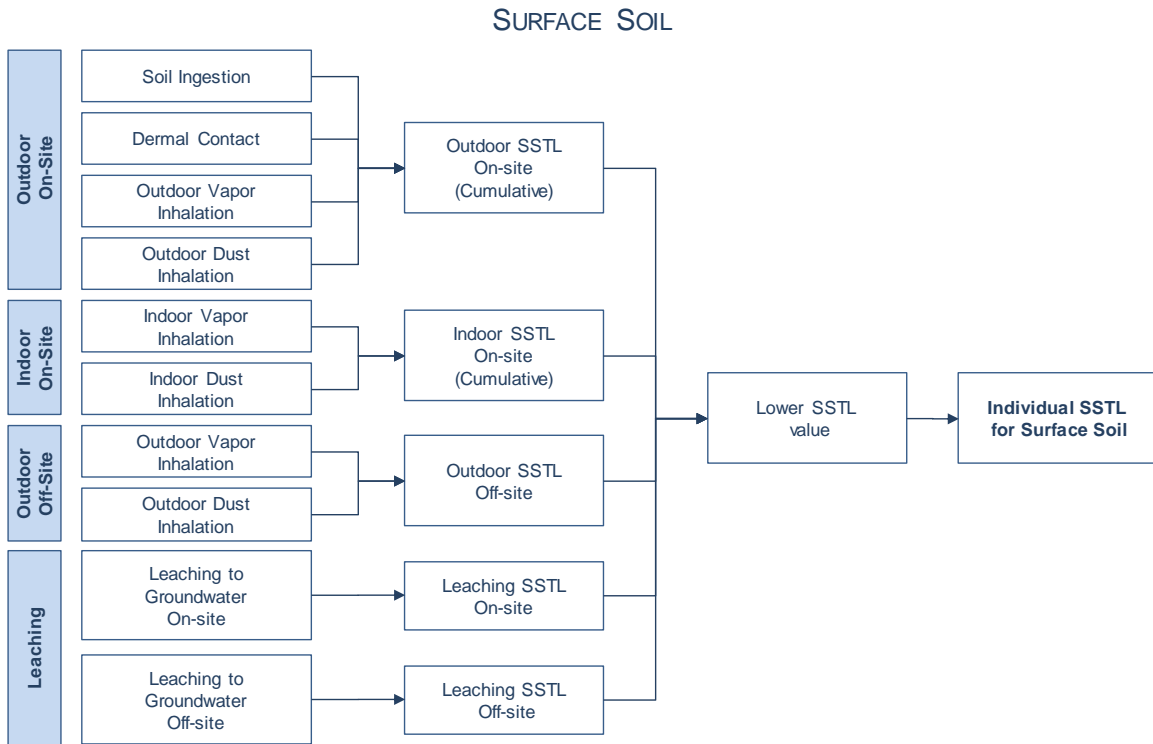


Figure 37. SSTL – Surface soil. Multiple exposures.

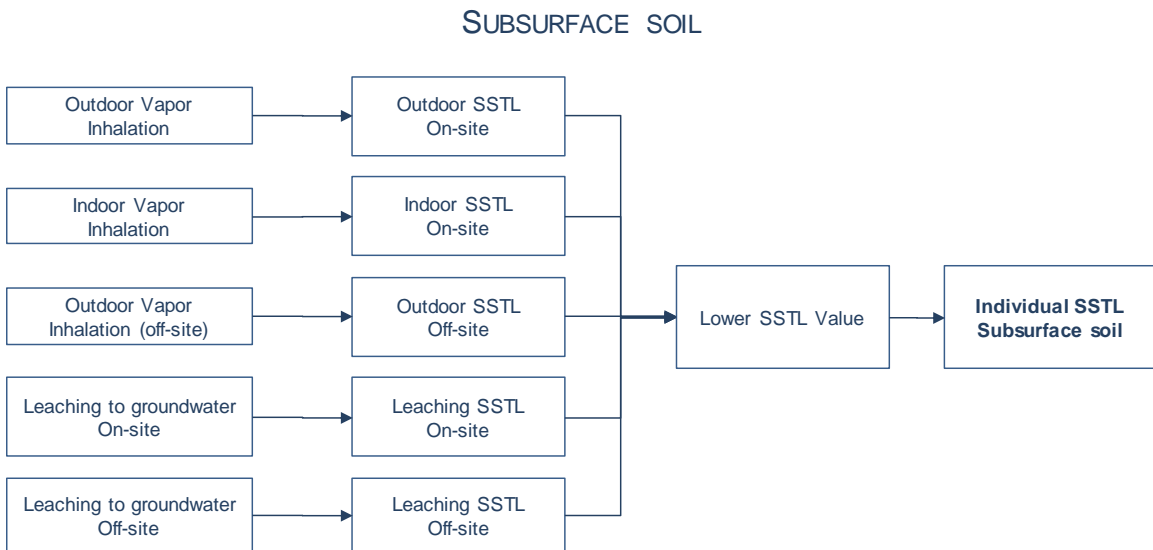


Figure 38. SSTL – Subsurface soil. Multiple exposures.

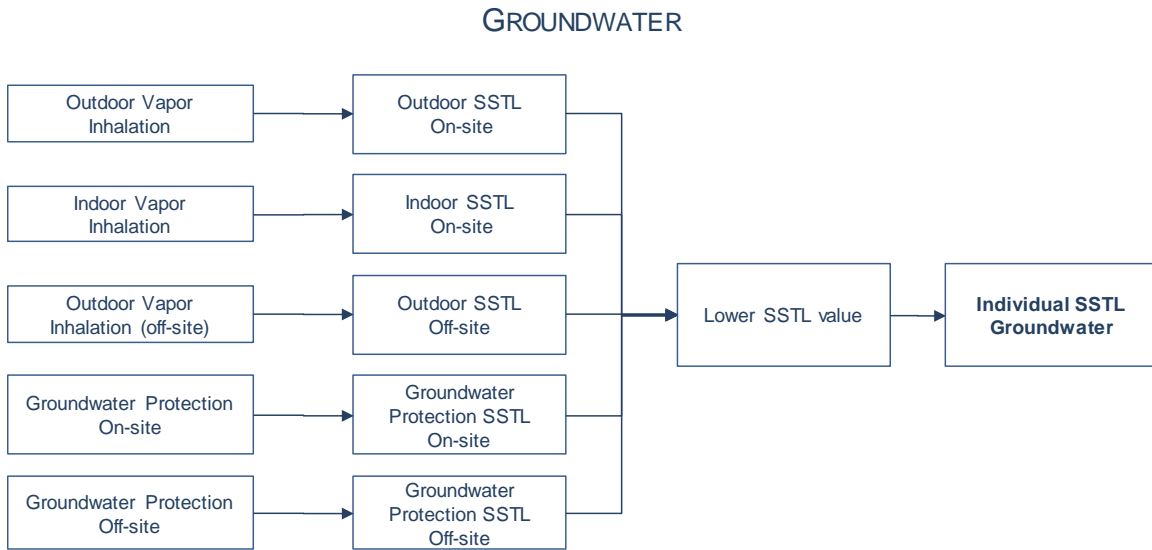


Figure 39. SSTL – Groundwater. Multiple exposures.

Cumulative SSTL (Clean-up levels). The SSTLs calculated above do not yet represent the final remediation targets, as they only ensure acceptable risk levels for exposure to individual contaminants. In fact, individual SSTLs may not satisfy cumulative risk criteria.

To account for cumulative risk effects, it is therefore necessary to further reduce the individual SSTLs to ensure that the resulting concentrations meet acceptable cumulative risk thresholds:

$$\sum_i^n SSTL_i^{cum} \cdot FT_i \cdot EM_i \cdot SF_i \leq TR \quad \text{for carcinogenic contaminants}$$

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

The SSTLs that satisfy both individual and cumulative risk criteria represent the final site-specific clean-up levels for the contaminated medium.

Table 22. Surface Soil: SSTL	
<p>Soil Ingestion (no off-site)</p> $SSTL_{SS.Ing} = \min \begin{cases} SSTL_{canc} = \frac{TR}{SF_{Ing} \cdot EM_{IngS} \cdot 10^{-6} \text{ kg/mg}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ing}}{EM_{IngS} \cdot 10^{-6} \text{ kg/mg}} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-canc} = SSTL non-carcinogenic TR = Target Risk THQ = Target Hazard Index SFI_{ng} = Slope factor - ingestion RfD_{Ing} = Reference dose - ingestion EM_{IngS} = Soil Ingestion rate</p>
<p>Dermal Contact (no off-site)</p> $SSTL_{SS.ConD} = \min \begin{cases} SSTL_{canc} = \frac{TR}{SF_{Ing} \cdot EM_{ConD} \cdot 10^{-6} \text{ kg/mg}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ing}}{EM_{ConD} \cdot 10^{-6} \text{ kg/mg}} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-canc} = SSTL non-carcinogenic TR = Target Risk THQ = Target Hazard Index SFI_{ng} = Slope factor - ingestion RfD_{Ing} = Reference dose - ingestion EM_{ConD} = Dermal contact rate</p>
<p>Outdoor Vapors Inhalation (reference dose method)</p> $SSTL_{SS.InaO} = \min \begin{cases} SSTL_{canc} = \frac{TR}{SF_{Ina} \cdot EM_{InaO} \cdot VF_{ss} \cdot ADF} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ina}}{EM_{InaO} \cdot VF_{ss} \cdot ADF} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-canc} = SSTL non-carcinogenic TR = Target Risk THQ = Target Hazard Index SFI_{na} = Slope factor - inhalation RfD_{Ina} = Reference dose – inhalation EM_{InaO} = Outdoor inhalation rate VF_{ss} = Outdoor Volatilization factor ADF = Atmospheric dispersion factor</p>
<p>Outdoor Vapors Inhalation (reference concentration method)</p> $SSTL_{SS.InaO} = \min \begin{cases} SSTL_{canc} = \frac{TR}{IUR_{Ina} \cdot EC_{InaO} \cdot VF_{ss} \cdot ADF} \\ SSTL_{non.canc} = \frac{THQ \cdot RfC_{Ina}}{EC_{InaO} \cdot VF_{ss} \cdot ADF} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-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</p>
<p>Outdoor Dusts Inhalation (reference dose method)</p> $SSTL_{SS.InaOP} = \min \begin{cases} SSTL_{canc} = \frac{TR}{SF_{Ina} \cdot EM_{InaO} \cdot PEF \cdot ADF} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ina}}{EM_{InaO} \cdot PEF \cdot ADF} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-canc} = SSTL non-carcinogenic TR = Target Risk THQ = Target Hazard Index SFI_{na} = Slope factor - inhalation RfD_{Ina} = Reference dose - inhalation EM_{InaO} = Outdoor inhalation rate PEF = Particulate emission factor ADF = Atmospheric dispersion factor</p>

Table 22. Surface Soil: SSTL	
<p>Outdoor Dusts Inhalation (reference concentration method)</p> $SSTL_{SS.InaOP} = \min \begin{cases} SSTL_{canc} = \frac{TR}{IUR_{Ina} \cdot EC_{InaO} \cdot PEF \cdot ADF} \\ SSTL_{non.canc} = \frac{THQ \cdot RfC_{Ina}}{EC_{InaO} \cdot PEF \cdot ADF} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non.canc} = SSTL non-carcinogenic TR = Target Risk THQ = Target Hazard Index SFI_{na} = Slope factor - inhalation RfD_{ina} = Reference dose - inhalation EM_{inaO} = Outdoor inhalation rate PEF = Particulate emission factor ADF = Atmospheric dispersion factor</p>
<p>Outdoor</p> $SSTL_{SS.outdoor} = \begin{cases} \frac{1}{\frac{1}{SSTL_{SS.IngS}} + \frac{1}{SSTL_{SS.ConD}} + \frac{1}{SSTL_{SS.InaO}} + \frac{1}{SSTL_{SS.InaOP}}} & (\text{for } SSTL_{InaO} \leq C_{sat}) \\ \frac{TR - R_{max,InaO}}{\frac{TR}{SSTL_{SS.IngS}} + \frac{TR}{SSTL_{SS.ConD}} + \frac{TR}{SSTL_{SS.InaOP}}} & (\text{for } SSTL_{InaO} > C_{sat}) \end{cases}$ $R_{max,InaO} = (C_{sat} / SSTL_{InaO}) \cdot TR \quad (\text{for } SSTL_{InaO} > C_{sat})$	
<p>Indoor Vapors Inhalation (no off-site) (reference dose method)</p> $SSTL_{SS.Inal} = \min \begin{cases} SSTL_{canc} = \frac{TR}{SF_{Ina} \cdot EM_{Inal} \cdot VF_{sresp}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ina}}{EM_{Inal} \cdot VF_{sresp}} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non.canc} = SSTL non-carcinogenic TR = Target Risk THQ = Target Hazard Index SFI_{na} = Slope factor - inhalation RfD_{ina} = Reference dose - inhalation EM_{inal} = Indoor inhalation rate VF_{sresp} = Indoor Volatilization factor</p>
<p>Indoor Vapors Inhalation (no off-site) (reference concentration method)</p> $SSTL_{SS.Inal} = \min \begin{cases} SSTL_{canc} = \frac{TR}{IUR_{Ina} \cdot EC_{Inal} \cdot VF_{sresp}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfC_{Ina}}{EC_{Inal} \cdot VF_{sresp}} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non.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 VF_{sresp} = Indoor Volatilization factor</p>
<p>Indoor Dusts Inhalation (no off-site) (reference dose method)</p> $SSTL_{SS.InalP} = \min \begin{cases} SSTL_{canc} = \frac{TR}{SF_{Ina} \cdot EM_{Inal} \cdot PEF_{in}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ina}}{EM_{Inal} \cdot PEF_{in}} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non.canc} = SSTL non-carcinogenic TR = Target Risk THQ = Target Hazard Index SFI_{na} = Slope factor - inhalation RfD_{ina} = Reference dose - inhalation EM_{inal} = Indoor inhalation rate PEF_{in} = Particulate indoor emission factor</p>

Table 22. Surface Soil: SSTL	
<p>Indoor Dusts Inhalation (no off-site) (reference concentration method)</p> $SSTL_{SS.InalP} = \min \begin{cases} SSTL_{canc} = \frac{TR}{IUR_{Ina} \cdot EC_{Inal} \cdot PEF_{in}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfC_{Ina}}{EC_{Inal} \cdot PEF_{in}} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non.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</p>
<p>Indoor</p> $SSTL_{SS.Indoor} = \begin{cases} \frac{1}{\frac{1}{SSTL_{SS.Inal}} + \frac{1}{SSTL_{SS.InalP}}} & (\text{for } SSTL_{Inal} \leq C_{sat}) \\ \frac{TR - R_{max,Inal}}{TR} \cdot SSTL_{SS.InalP} & (\text{for } SSTL_{Inal} > C_{sat}) \end{cases}$ <p>$R_{max,Inal} = (C_{sat} / SSTL_{Inal}) \cdot TR$ (for $SSTL_{Inal} > C_{sat}$)</p>	
<p>Leaching to groundwater</p> $SSTL_{SS.LF} = \min \begin{cases} SSTL_{canc} = \frac{TR \cdot DAF}{SF_{Ing} \cdot EM_{IngW} \cdot LF_{ss}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ing} \cdot DAF}{EM_{IngW} \cdot LF_{ss}} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non.canc} = SSTL non-carcinogenic TR = Target Risk THQ = Target Hazard Index SF_{Ing} = Slope factor - ingestion RfD_{Ing} = Reference dose - ingestion EM_{IngW} = Water ingestion rate LF_{ss} = Leaching Factor DAF = Groundwater dilution factor</p>
<p>SSTL – Surface Soil</p> $SSTL_{SS} = \min [SSTL_{SS.outdoor}; SSTL_{SS.Indoor}; SSTL_{SS.LF}]$	

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

Table 23. Subsurface Soil: SSTL	
<p>Outdoor Vapors Inhalation (reference dose method)</p> $SSTL_{SP.InaO} = \min \begin{cases} SSTL_{canc} = \frac{TR}{SF_{Ina} \cdot VF_{samb} \cdot EM_{InaO} \cdot ADF} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ina}}{VF_{samb} \cdot EM_{InaO} \cdot ADF} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-canc} = SSTL non-carcinogenic cont. TR = Target Risk THQ = Target Hazard Index SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose – inhalation EM_{InaO} = Outdoor inhalation rate VF_{samb} = Outdoor Volatilization factor ADF = Atmospheric dispersion factor</p>
<p>Outdoor Vapors Inhalation (reference concentration method)</p> $SSTL_{SP.InaO} = \min \begin{cases} SSTL_{canc} = \frac{TR}{IUR_{Ina} \cdot VF_{samb} \cdot EC_{InaO} \cdot ADF} \\ SSTL_{non.canc} = \frac{THQ \cdot RfC_{Ina}}{VF_{samb} \cdot EC_{InaO} \cdot ADF} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-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</p>
<p>Indoor Vapors Inhalation (no off-site) (reference dose method)</p> $SSTL_{SP.Inal} = \min \begin{cases} SSTL_{canc} = \frac{TR}{SF_{Ina} \cdot VF_{seps} \cdot EM_{Inal}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ina}}{VF_{seps} \cdot EM_{Inal}} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-canc} = SSTL non-carcinogenic cont. TR = Target Risk THQ = Target Hazard Index SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose – inhalation EM_{Inal} = Indoor inhalation rate VF_{seps} = Indoor Volatilization factor</p>
<p>Indoor Vapors Inhalation (no off-site) (reference concentration method)</p> $SSTL_{SP.Inal} = \min \begin{cases} SSTL_{canc} = \frac{TR}{IUR_{Ina} \cdot VF_{seps} \cdot EC_{Inal}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfC_{Ina}}{VF_{seps} \cdot EC_{Inal}} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-canc} = SSTL non-carcinogenic cont. TR = Target Risk THQ = Target Hazard Index IUR_{Ina} = Inhalation Unit Risk RfC_{Ina} = Reference concentration EC_{Inal} = Indoor inhalation rate VF_{seps} = Indoor Volatilization factor</p>
<p>Leaching to groundwater</p> $SSTL_{SP.LF} = \min \begin{cases} SSTL_{canc} = \frac{TR \cdot DAF}{SF_{Ing} \cdot EM_{IngW} \cdot LF_{sp}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ing} \cdot DAF}{EM_{IngW} \cdot LF_{sp}} \end{cases}$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-canc} = SSTL non-carcinogenic cont. TR = Target Risk THQ = Target Hazard Index SF_{Ing} = Slope factor - ingestion RfD_{Ing} = Reference dose - ingestion EM_{IngW} = Water ingestion rate LF_{sp} = Leaching factor DAF = Groundwater dilution factor</p>
<p>SSTL – Subsurface Soil</p> $SSTL_{SP} = \min [SSTL_{SP.InaO}; SSTL_{SP.Inal}; SSTL_{SP.LF}]$	

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

Table 24. Groundwater: SSTL	
<p>Outdoor Vapors Inhalation (reference dose method)</p> $SSTL_{GW.InaO} = \min \left\{ \begin{array}{l} SSTL_{canc} = \frac{TR \cdot DAF}{SF_{Ina} \cdot VF_{wamb} \cdot EM_{InaO}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ina} \cdot DAF}{VF_{wamb} \cdot EM_{InaO}} \end{array} \right.$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-canc} = SSTL non-carcinogenic cont. TR = Target Risk THQ = Target Hazard Index SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose – inhalation EM_{InaO} = Outdoor inhalation rate VF_{wamb} = Outdoor Volatilization factor DAF = Groundwater dilution factor</p>
<p>Outdoor Vapors Inhalation (reference concentration method)</p> $SSTL_{GW.InaO} = \min \left\{ \begin{array}{l} SSTL_{canc} = \frac{TR \cdot DAF}{IUR_{Ina} \cdot VF_{wamb} \cdot EC_{InaO}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfC_{Ina} \cdot DAF}{VF_{wamb} \cdot EC_{InaO}} \end{array} \right.$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-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</p>
<p>Indoor Vapors Inhalation (reference dose method)</p> $SSTL_{GW.Inal} = \min \left\{ \begin{array}{l} SSTL_{canc} = \frac{TR \cdot DAF}{SF_{Ina} \cdot VF_{wesp} \cdot EM_{Inal}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ina} \cdot DAF}{VF_{wesp} \cdot EM_{Inal}} \end{array} \right.$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-canc} = SSTL non-carcinogenic cont. TR = Target Risk THQ = Target Hazard Index SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose – inhalation EM_{Inal} = Indoor inhalation rate VF_{wesp} = Indoor Volatilization factor DAF = Groundwater dilution factor</p>
<p>Indoor Vapors Inhalation (reference concentration method)</p> $SSTL_{GW.Inal} = \min \left\{ \begin{array}{l} SSTL_{canc} = \frac{TR \cdot DAF}{IUR_{Ina} \cdot VF_{wesp} \cdot EC_{Inal}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfC_{Ina} \cdot DAF}{VF_{wesp} \cdot EC_{Inal}} \end{array} \right.$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-canc} = SSTL non-carcinogenic cont. TR = Target Risk THQ = Target Hazard Index IUR_{Ina} = Inhalation Unit Risk RfC_{Ina} = Reference concentration EC_{Inal} = Indoor inhalation rate VF_{wesp} = Indoor Volatilization factor DAF = Groundwater dilution factor</p>
<p>Water Ingestion</p> $SSTL_{GW.D} = \min \left\{ \begin{array}{l} SSTL_{canc} = \frac{TR \cdot DAF}{SF_{Ing} \cdot EM_{IngW}} \\ SSTL_{non.canc} = \frac{THQ \cdot RfD_{Ing} \cdot DAF}{EM_{IngW}} \end{array} \right.$	<p>SSTL_{canc} = SSTL carcinogenic cont. SSTL_{non-canc} = SSTL non-carcinogenic cont. TR = Target Risk THQ = Target Hazard Index SF_{Ing} = Slope factor - ingestion RfD_{Ing} = Reference dose - ingestion EM_{IngW} = Water ingestion rate DAF = Groundwater dilution factor</p>
<p>SSTL - Groundwater $SSTL_{GW} = \min [SSTL_{GW.InaO}; SSTL_{GW.Inal}; SSTL_{GW.D}]$</p>	

For On-site Receptors DAF = 1

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

For On-site Receptors DAF = 1

Table 26. SSTL: TPH Mixtures

MADEP CLASSIFICATION

Hydrocarbons C < 12

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

Hydrocarbons C > 12

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

Total Hydrocarbons

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

Nomenclature

$SSTL_{MADEPi}$ = 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

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

Hydrocarbons C > 12

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

Total Hydrocarbons

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

Nomenclature

$SSTL_{TPHi}$ = 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 TPH class for total hydrocarbons

Table 27. Screening for free phase migration (NAPL)

Vadose zone (ASTM E2081-00)

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

Saturated Zone (ASTM E2081-00)

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

Residual phase volume fraction, θ_o (-)

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

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/cm³)

ρ_o = Contaminant density (g/cm³)

APP. 2B. REFERENCE CONCENTRATIONS

Table 28. Reference Concentration (CR): air	
<p>Outdoor Vapors Inhalation (reference dose method)</p> $CR_{AR.InaO} = \min \begin{cases} CR_{canc} = \frac{TR}{SF_{Ina} \cdot EM_{InaO} \cdot ADF} \\ CR_{non.canc} = \frac{THQ \cdot RfD_{Ina}}{EM_{InaO} \cdot ADF} \end{cases}$	<p>CR_{canc} = CR carcinogenic cont. CR_{non-canc} = CR non-carcinogenic cont TR = Target Risk THQ = Target Hazard Index SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose – inhalation EM_{InaO} = Outdoor inhalation rate ADF = Atmospheric dispersion factor</p>
<p>Outdoor Vapors Inhalation (reference concentration method)</p> $CR_{AR.InaO} = \min \begin{cases} CR_{canc} = \frac{TR}{IUR \cdot EC_{InaO} \cdot ADF} \\ CR_{non.canc} = \frac{THQ \cdot RfC}{EC_{InaO} \cdot ADF} \end{cases}$	<p>CR_{canc} = CR carcinogenic cont. CR_{non-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</p>
<p>Indoor Vapors Inhalation (reference dose method)</p> $CR_{AR.Inal} = \min \begin{cases} CR_{canc} = \frac{TR}{SF_{Ina} \cdot EM_{Inal}} \\ CR_{non.canc} = \frac{THQ \cdot RfD_{Ina}}{EM_{Inal}} \end{cases}$	<p>CR_{canc} = CR carcinogenic cont. CR_{non-canc} = CR non-carcinogenic cont TR = Target Risk THQ = Target Hazard Index SF_{Ina} = Slope factor - inhalation RfD_{Ina} = Reference dose – inhalation EM_{Inal} = Indoor inhalation rate</p>
<p>Indoor Vapors Inhalation (reference concentration method)</p> $CR_{AR.Inal} = \min \begin{cases} CR_{canc} = \frac{TR}{IUR \cdot EC_{Inal}} \\ CR_{non.canc} = \frac{THQ \cdot RfC}{EC_{Inal}} \end{cases}$	<p>CR_{canc} = CR carcinogenic cont. CR_{non-canc} = CR non-carcinogenic cont TR = Target Risk THQ = Target Hazard Index IUR = Inhalation Unit Risk EC_{Inal} = Indoor inhalation rate</p>
<p>CR air $CR_{AR} = \min [CR_{AR.InaO}; CR_{AR.Inal}]$</p>	

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	
$CR_{SG.Inal} = \frac{CR_{AR.Inal}}{\alpha_{seep}}$	α_{seep} = Indoor volatilization factor
CR soil-gas	
$CR_{SG} = \min [CR_{SG.InaO}; CR_{SG.Inal}]$	

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	
$CR_{ELss} = \min \left\{ \begin{array}{l} CR_{canc} = \frac{TR \cdot DAF}{SF_{Ing} \cdot EM_{IngW} \cdot \alpha_{LFss}} \\ CR_{non.canc} = \frac{THQ \cdot RfD_{Ing} \cdot DAF}{EM_{IngW} \cdot \alpha_{LFss}} \end{array} \right.$	CR_{canc} = CR carcinogenic cont. $CR_{non.canc}$ = CR non-carcinogenic cont TR = Target Risk THQ = Target Hazard Index SF_{Ing} = Slope factor - ingestion RfD_{Ing} = 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	
<p>Groundwater Protection</p> $CR_{ELsp} = \frac{MCL_{GW} \cdot DAF}{\alpha_{LFsp}}$	<p>MCL = Maximum contaminant level α_{LFsp} = Leaching factor DAF = Dilution attenuation factor</p>
<p>Water Ingestion</p> $CR_{ELsp} = \min \left\{ \begin{array}{l} CR_{canc} = \frac{TR \cdot DAF}{SF_{Ing} \cdot EM_{IngW} \cdot \alpha_{LFsp}} \\ CR_{non.canc} = \frac{THQ \cdot RfD_{Ing} \cdot DAF}{EM_{IngW} \cdot \alpha_{LFsp}} \end{array} \right.$	<p>CR_{canc} = CR carcinogenic cont. CR_{non-canc} = CR non-carcinogenic cont TR = Target Risk THQ = Target Hazard Index SF_{Ing} = Slope factor - ingestion RfD_{Ing} = Reference dose – ingestion EM_{IngW} = Outdoor ingestion rate α_{LFsp} = Leaching factor DAF = Dilution attenuation factor</p>

For On-site Receptors DAF=1

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

Fate and transport factors (F&T) are used in the assessment of indirect exposure pathways, where contaminants reach receptors through migration and diffusion from the environmental compartment.

The calculation of transport factors requires the definition of both the physical characteristics of the affected environmental media (vadose zone, groundwater, indoor and outdoor air) and the physico-chemical properties of the contaminants, in order to evaluate their distribution and dispersion.

The fate and transport factors considered in the software are the following:

From Surface Soil

- VF_{ss} : Outdoor volatilization factor
- VF_{seps} : 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_{seps} : 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 underlying the equations are as follows:

- The concentration of contaminants in soil is uniformly distributed and remains constant over the entire exposure period;
- The soil is assumed to be homogeneous, isotropic, and unconsolidated;
- No biodegradation (except for DAF) or other degradation/transformation processes of contaminants are considered.

Table 33. Surface Soil: Outdoor vapor volatilization

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

Optional check

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

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 (cm²/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/cm³)
- BDF_{Vol} = Biodegradation factor (-)

Table 34. Surface Soil: Indoor vapor volatilization

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

No differential outdoor/indoor pressure ($\Delta p=0$)

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

Differential outdoor/indoor pressure ($\Delta p \neq 0$)

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

Convective Air Flow Through Foundation Cracks, Q_s (cm³/s)

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

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 (cm²/s)
- D_{crack}^{eff} = Effective diffusivity in the foundations (cm²/s)
- T_{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/cm³)
- X_{crack} = Enclosed space foundation perimeter (cm)
- Δp = Differential indoor/outdoor air pressure (g/cm²/s)
- k_v = Soil vapor permeability (cm²)
- A_b = Area of building foundation (cm²)
- μ_{air} = Vapor Viscosity (g/cm/s)
- BDF_{Vol} = Biodegradation factor (-)

Table 35. Surface Soil: Leaching Factor

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

Soil Attenuation model, SAM (-)

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

Dilution Factor, LDF (-)

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

Partition Coefficient (kg/L)

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

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

$$\delta_{gw} = (2 \cdot 0.0056 \cdot W^2)^{0.5} + d_a \cdot \left[1 - \exp \left(- \frac{W \cdot I_{eff}}{v_{gw} \cdot d_a} \right) \right] \quad \text{for } \delta_{gw} > d_a \rightarrow \delta_{gw} = d_a$$

Infiltration Rate (Optional)

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

Sandy Soils (Sand, Loamy Sand and SandyLoam) $\beta = 0.0018$; Silty Soils (Sandy Clay Loam, Loam, Silt Loam and Silt) $\beta = 0.0009$; Clay Soils (Clay Loam, Silty Clay Loam, Silty Clay, Sandy Clay and Clay) $\beta = 0.00018$.

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/cm³)
- 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/cm²/s)

F_i = 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 [cm³/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	σ_y (m)	σ_z (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 $100\text{ m} < d < 10000\text{ m}$

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 (δ_{air})

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

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

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

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 (cm²/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/cm³)
- BDF_{Vol} = Biodegradation factor (-)

Table 41. Subsurface Soil: Indoor vapor volatilization

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

No differential outdoor/indoor pressure ($\Delta p=0$)

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

Differential outdoor/indoor pressure ($\Delta p \neq 0$)

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

Convective Air Flow Through Foundation Cracks, Q_s (cm³/s)

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

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 (cm²/s)
- D_{crack}^{eff} = Effective diffusivity in the foundations (cm²/s)
- T_{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/cm³)
- X_{crack} = Enclosed space foundation perimeter (cm)
- Δp = Differential indoor/outdoor air pressure (g/cm²/s)
- k_v = Soil vapor permeability (cm²)
- A_b = Area of building foundation (cm²)
- μ_{air} = Vapor Viscosity (g/cm/s)
- BDF_{Vol} = Biodegradation factor (-)

Table 42. Subsurface Soil: Leaching Factor

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

Soil Attenuation model, SAM (-)

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

Dilution Factor, LDF (-)

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

Partition Coefficient (kg/L)

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

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

$$\delta_{gw} = (2 \cdot 0.0056 \cdot W^2)^{0.5} + d_a \cdot \left[1 - \exp \left(- \frac{W \cdot I_{eff}}{v_{gw} \cdot d_a} \right) \right] \quad \text{for } \delta_{gw} > d_a \rightarrow \delta_{gw} = d_a$$

Infiltration Rate

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

Sandy Soils (Sand, Loamy Sand and SandyLoam) $\beta = 0.0018$; Silty Soils (Sandy Clay Loam, Loam, Silt Loam and Silt) $\beta = 0.0009$; Clay Soils (Clay Loam, Silty Clay Loam, Silty Clay, Sandy Clay and Clay) $\beta = 0.00018$.

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/cm³)
 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 (-)

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

DAF2 (-)

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

DAF3(-)

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

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/cm³)

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 ($\Delta p=0$)

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

Differential outdoor/indoor pressure ($\Delta p \neq 0$)

$$VF_{wesp} \left[\frac{mg / m^3_{air}}{mg / L_{water}} \right] = \frac{H \cdot \frac{D_w^{eff}}{(L_{gw} - Z_{crack}) L_b \cdot ER} \cdot e^{\xi}}{e^{\xi} + \frac{D_w^{eff}}{(L_{gw} - Z_{crack}) L_b \cdot ER} + \frac{D_w^{eff} \cdot A_b}{Q_s \cdot (L_{gw} - Z_{crack})}} \cdot BDF_{Vol} \cdot 10^3$$

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

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

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)
- T_{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

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

Nomenclature

L_{gw} = Depth to Groundwater (cm)

D_w^{eff} = Effective diffusivity from groundwater (cm²/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

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

Diffusion Coefficient in the presence of a clay lens

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

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 (cm²/s)
- D_w = Diffusion coefficient in water (cm²/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/cm³)

Table 47. Saturation Concentration (C_{sat})

Saturation Concentration

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

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/cm³)

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

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

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 (cm^2/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

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

Nomenclature

L_s = Depth of the source (cm) *
 D_s^{eff} = Effective diffusivity in the vadose zone (cm^2/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)

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

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)

h_{cr} = Wetting front suction (matric potential) (cm)

θ_e = Effective porosity in the unsaturated zone (-)

K_s = Partition Coefficient (mg/kg/mg/L)

ρ_s = Soil bulk density (g/cm³)

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) $\beta = 0.0018$; Silty Soils (Sandy Clay Loam, Loam, Silt Loam and Silt) $\beta = 0.0009$; Clay Soils (Clay Loam, Silty Clay Loam, Silty Clay, Sandy Clay and Clay) $\beta = 0.00018$.

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 (cm²)
 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 (#/cm²)
 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
- $PEF_{MdR,in}$: Indoor particulate emission
- LF_{MdR} : Leaching factor

Air Dispersion

- ADF : Air Dispersion Factor

Table 51. Backfill Material: Outdoor vapor volatilization

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

Optional check

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

Nomenclature

- d_{Mdr} = Thickness of backfill material (cm)
- L_{Mdr} = Depth to backfill material (cm)
- D_{Mdr}^{eff} = Effective diffusivity in the backfill material (cm²/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/cm³)
- BDF_{Vol} = Biodegradation factor (-)

Table 52. Backfill Material: Indoor vapor volatilization

$$VF_{Mdr,esp} \left[\frac{mg / m^3_{air}}{mg / kg_{soil}} \right] = \min \left\{ \begin{array}{l} VF_{Mdr,esp} (1) \\ VF_{Mdr,esp} (2) = \frac{\rho_{Mdr} \cdot d_{Mdr}}{L_b \cdot ER \cdot \tau_{indoor}} 10^3 \quad (\text{optional}) \end{array} \right.$$

No differential outdoor/indoor pressure ($\Delta p=0$)

$$VF_{Mdr,esp} (1) = \frac{\frac{H \cdot \rho_{Mdr}}{(\theta_{w,Mdr} + K_{s,Mdr} \cdot \rho_{Mdr} + H \cdot \theta_{a,Mdr})} \cdot \frac{D_{Mdr}^{eff}}{(L_{Mdr} - Z_{crack}) \cdot L_b \cdot ER}}{1 + \frac{D_{Mdr}^{eff}}{(L_{Mdr} - Z_{crack}) \cdot L_b \cdot ER} + \frac{D_{Mdr}^{eff} \cdot L_{crack}}{D_{crack}^{eff} \cdot \eta \cdot (L_{Mdr} - Z_{crack})}} BDF_{Vol} \cdot 10^3$$

Differential outdoor/indoor pressure ($\Delta p \neq 0$)

$$VF_{Mdr,esp} (1) = \frac{\frac{H \cdot \rho_{Mdr}}{(\theta_{w,Mdr} + K_{s,Mdr} \cdot \rho_{Mdr} + H \cdot \theta_{a,Mdr})} \cdot \frac{D_{Mdr}^{eff}}{(L_{Mdr} - Z_{crack}) \cdot L_b \cdot ER} \cdot e^{\xi}}{e^{\xi} + \frac{D_{Mdr}^{eff}}{(L_{Mdr} - Z_{crack}) \cdot L_b \cdot ER} + \frac{D_{Mdr}^{eff} \cdot A_b}{Q_s \cdot (L_{Mdr} - Z_{crack})} \cdot (e^{\xi} - 1)} BDF_{Vol} \cdot 10^3$$

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

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

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}^{eff} = 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/cm²/s)

F_i = 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 [cm³/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

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

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

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

Leachate Dilution Factor, LDF (-)

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

Partition coefficients (kg/L)

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

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

$$\delta_{gw} = (2 \cdot 0.0056 \cdot W^2)^{0.5} + d_a \cdot \left[1 - \exp \left(- \frac{W \cdot I_{eff,Mdr}}{v_{gw} \cdot d_a} \right) \right] \quad \text{Se } \delta_{gw} > d_a \rightarrow \delta_{gw} = d_a$$

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/cm³)
- 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 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 (cm²/s)
- D_w = Diffusion coefficient in water (cm²/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

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

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/cm³)
- f_{oc} = Organic Carbon Fraction (-)
- S = solubility (mg/L)
- H = Henry's law constant (-)

Table 58. Eluate Backfill Materials: Leachate

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

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

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

Leachate Dilution Factor, LDF (-)

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

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

$$\delta_{gw} = (2 \cdot 0.0056 \cdot W^2)^{0.5} + d_a \cdot \left[1 - \exp \left(- \frac{W \cdot I_{eff}}{v_{gw} \cdot d_a} \right) \right] \quad \text{Se } \delta_{gw} > d_a \rightarrow \delta_{gw} = d_a$$

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)

T_{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/cm³)

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

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

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

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

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

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

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)
- T_{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/cm³)
- 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

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

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

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

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)
- T_{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/cm³)
- 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 (-)

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_{seps} : indoor volatilization factor

Flux chamber

- α_{FC} : outdoor volatilization factor (open flux chamber)
- $\alpha_{\text{FC(flux)}}$: 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 underlying the equations are as follows:

- The concentration of contaminants in soil is uniformly distributed and remains constant over the entire exposure period;
- The soil is assumed to be homogeneous, isotropic, and unconsolidated;

No biodegradation (except for DAF) or other degradation/transformation processes of contaminants are considered.

Table 60. Soil-gas: Outdoor Volatilization

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

Nomenclature

- L_{sg} = Soil Gas Probe Depth (cm)
- D_s^{eff} = Effective diffusivity in the vadose zone (cm²/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)

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

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)
- Q_{in} = Flowrate of the carrier gas in the chamber (cm³/s)
- A_{fc} = Chamber surface exposed to soil (cm²)

Open and closed flux chamber (Input: Flux)

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

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 ($\Delta p=0$)

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

Differential outdoor/indoor pressure ($\Delta p \neq 0$)

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

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

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

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)
- T_{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)

Q_{in} = Flowrate of the carrier gas in the chamber (cm³/s)

A_{fc} = Chamber surface exposed to soil (cm²)

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 (-)

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

Leachate Dilution Factor, LDF (-)

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

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

$$\delta_{gw} = (2 \cdot 0.0056 \cdot W^2)^{0.5} + d_a \cdot \left[1 - \exp\left(-\frac{W \cdot I_{eff}}{v_{gw} \cdot d_a}\right) \right] \quad \text{If } \delta_{gw} > d_a \rightarrow \delta_{gw} = d_a$$

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 (-)

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

Leachate Dilution Factor, LDF (-)

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

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

$$\delta_{gw} = (2 \cdot 0.0056 \cdot W^2)^{0.5} + d_a \cdot \left[1 - \exp\left(-\frac{W \cdot I_{eff}}{v_{gw} \cdot d_a}\right) \right] \quad \text{If } \delta_{gw} > d_a \rightarrow \delta_{gw} = d_a$$

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).

<p>Dermal Contact</p> $EM \left[\frac{mg}{kg \times day} \right] = \frac{SA \cdot AF \cdot ABS \cdot EF \cdot ED}{BW \cdot AT \cdot 365} \frac{days}{year}$	<p>BW = Body weight (kg) EF = Exposure frequency (d/year) ED = Exposure Duration (years) AT = Averaging time (years) (*) SA = Skin Surface Area (cm²) AF = Soil Dermal adherence factor (mg/(cm² d)) ABS = Dermal adsorption factor (-)</p>
<p>Soil ingestion</p> $EM \left[\frac{mg}{kg \times day} \right] = \frac{IR \cdot FI \cdot EF \cdot ED}{BW \cdot AT \cdot 365} \frac{days}{year}$	<p>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 (-)</p>
<p>Outdoor Vapors and Dust Inhalation</p> $EM \left[\frac{m^3}{kg \times day} \right] = \frac{B_o \cdot EF_{go} \cdot EF \cdot ED}{BW \cdot AT \cdot 365} \frac{days}{year}$	<p>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 (m³/h)</p>
<p>Indoor Vapors and Dust Inhalation</p> $EM \left[\frac{m^3}{kg \times day} \right] = \frac{B_i \cdot EF_{gi} \cdot EF \cdot ED}{BW \cdot AT \cdot 365} \frac{days}{year}$	<p>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 (m³/h)</p>
<p>Water Ingestion</p> $EM \left[\frac{L}{kg \times day} \right] = \frac{IR_w \cdot EF \cdot ED}{BW \cdot AT \cdot 365} \frac{days}{year}$	<p>BW = Body weight (kg) EF = Exposure frequency (d/year) ED = Exposure Duration (years) AT = Averaging time (years) (*) IR_w = Water Ingestion rate (L/d)</p>

(*) For non-carcinogenic contaminants AT = ED

APP. 5. USING ADVANCED CHARACTERIZATION DATA

By default, data obtained from advanced site characterization (soil gas, flux chamber measurements, air measurements, and leaching tests) are used exclusively for risk estimation for receptors. However, through the “Model options” (specifically the “Advanced Characterization” screen), the user can choose to also use these data to refine the estimation of SSTLs for the different environmental media (surface soil, subsurface soil, and groundwater).

In this case, data from monitoring campaigns are used to derive semi-empirical transport factors for the selected sources, which are then applied to update the SSTLs. The calculation of empirical and semi-empirical transport factors is described in the following sections.

Outdoor air measurements

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

This attenuation factor, denoted as β , can be estimated for soil and groundwater using the following equations:

Volatilization from soil

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

Volatilization from groundwater

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

where:

$C_{air,outdoor}$ = Ambient Air Concentration (mg/m³)

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 outdoor air. Once the site-specific β factors have been derived from monitoring data, they can be used to estimate site-specific transport factors, which are then applied in the standard equations for SSTL calculation.

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 also be used to estimate site-specific vapor attenuation. By comparing concentrations measured indoors with those in the source, the attenuation between the source and the indoor environment can be evaluated.

The attenuation factor β can be estimated 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/m³)

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

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

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

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 evaluate vapor attenuation between the source and the sampling depth. By comparing soil-gas concentrations with source concentrations, it is possible to estimate attenuation during subsurface transport.

The attenuation factor β is calculated as follows:

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:

$C_{soil-gas}$ = 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 chamber data can be used to assess vapor attenuation from the source to the ground surface. By measuring concentrations in the chamber and in the source, attenuation during upward migration can be estimated.

The attenuation factor β can be calculated for soil and groundwater using:

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/m³)

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)

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

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

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

Leaching test results can be used to evaluate site-specific partitioning between contaminants in the source and those in the dissolved phase. By comparing concentrations in eluate with those in soil or groundwater, it is possible to estimate the partitioning behavior of contaminants.

The attenuation factor β is calculated as follows:

Eluate – Surface Soil

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

Eluate – Subsurface Soil

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

where:

$C_{eluate,ss}$ = Concentration in the eluate of the leaching test carried out on the surface soil (mg/L)

C_{ss} = Concentration in surface soil (mg/kg)

$C_{eluate,sp}$ = 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 review the expected concentrations in soil gas, eluate, outdoor air, and indoor air, based on the source concentrations defined by the user (surface soil, subsurface soil, or groundwater).

This appendix presents the equations used by the software to perform these estimations.

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

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

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/m³)

$C_{Air.Indoor}$: concentration expected in indoor air (mg/m³)

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*

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

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

From Subsurface Soil

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

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

From Groundwater

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

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

Nomenclature

$C_{sg,Outdoor}$: concentration expected in the soil gas for the outdoor volatilization pathway (mg/m³)

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*

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

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

From Subsurface Soil

$$C_{sg, Indoor(sp)} = C_{sp} \cdot \frac{VF_{seep}}{\alpha_{seep}}$$

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

From Groundwater

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

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

Nomenclature

$C_{sg, Indoor}$: concentration expected in the soil gas for the indoor volatilization pathway (mg/m³)

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/m³)**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*

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

From Subsurface Soil

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

Nomenclature*C_{EI}: 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 acting through a genotoxic mechanism, the software allows the application of an adjustment factor (ADAF, Age-Dependent Adjustment Factor) to the carcinogenic toxicological parameters (SF Ing., SF Inal., IUR), depending on 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, ADAF values are defined for specific contaminants. In particular, for benzo(a)pyrene, dibenzo(a,h)anthracene, 1,2,3-trichloropropane, dichloromethane, trichloroethylene, and acrylamide, an ADAF of 5 is applied for children and 3 for teenagers. For vinyl chloride, the ADAF for children is set to 2.

APP. 8. KOC AND KD FUNCTION OF PH

For substances for which Koc and Kd depend on pH, when the default database is used, the software adopts the distribution coefficient values reported in the following tables, based on the pH defined for 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

App. 8. Koc and Kd function of pH

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