Distribution: General

S-Risk user manual

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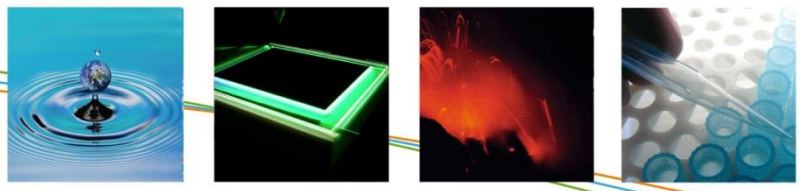

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REVISIONS

Date	Modification
25/02/2014	4.6.1 – last paragraph before title 'Tier 1' – explanation added on the difference between the options 'gaps and holes' and 'intact floor' 4.6.1 – Tier 2 – information added in parameter table on what is represented by the default values related to floor and wall quality
04/11/2015	Correction of typing errors and inconsistencies. Update of paragraphs 4.13, 5.2 and 6.6 about new facilities (i.e., online result summary) on Results tab. Addition of paragraphs 4.14, 5.3 and 6.7 on Graph tab.
05/08/2016	Modifications in function of release 1.1.4(.3) and 1.1.5: - Update of paragraph 4.1.1 about default land use settings, paragraph 4.7 about Plants tab and paragraphs 5.2 and 6.6 about new optimization algorithm on Results tab; - Addition of new paragraph 4.10.2 about visibility of food consumption figures on Exposure tab; - Removing of paragraph 5.3 about Graph tab.
24/11/2016	Modifications in function of release 1.2.1: - Addition of information about new archiving functionality to paragraphs 3.1.1, 3.1.3 and 3.3; - Addition of information about the different S-Risk regions/version at sever places in the manual; - Update of warning message about adding basement air measurements in paragraph 4.9.3.
06/02/2016	4.14 – Explication of coloured lines added for Graph tab functionality.
14/03/2017	Modification in function of release 1.2.2: addition of information about depth groundwater table and depth building+buffer space to paragraphs 4.3.1 and 4.6.1
04/12/2017	Modification in function of releases 1.2.3 and 1.2.4: addition of information about online result summary to paragraph 4.13.

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CHAPTER 1 INTRODUCTION

This document describes the use of the S-Risk web application version 1.2.4. Guidance with regard to the user interface and several model parameters is provided by means of screenshots and clarifying text. Detailed information on model concepts and parameterization can be found in the Technical Guidance document. Additional information regarding theoretical and practical topics can be found on the FAQ page as well.

CHAPTER 2 LOGGING IN TO S-RISK

S-Risk is accessible through the internet. You can login after starting up one of the internet browsers that are supported by the software (Internet Explorer 9 or higher, FireFox 19 or higher or Google Chrome) and entering the URL https://www.s-risk.be. The S-Risk homepage will appear.

After clicking the **S-Risk Application tab**, you will be redirected to the S-Risk login page (Figure 1), which provides an SSL secured connection to protect your login details.

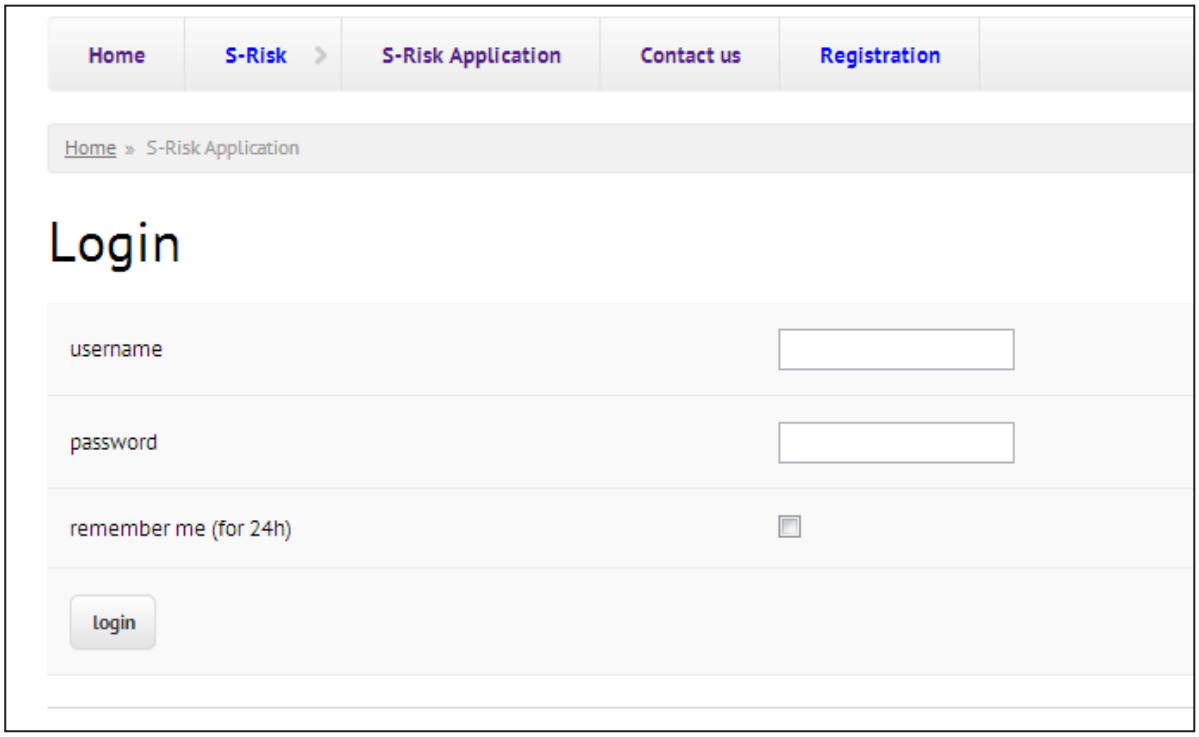


Figure 1: The S-Risk login page

On this page, you can log in with the username and password you received for a certain region after registration. Logging in will activate a new session. Your session expires automatically after an inactivity period of 30 minutes after which you will need to log in again, except if you activated the check box for the remember me option. In that case your login data are saved by the system for 24 h.

The system does not allow more than one simultaneous session per account. In that case you will receive an error message (Figure 2).

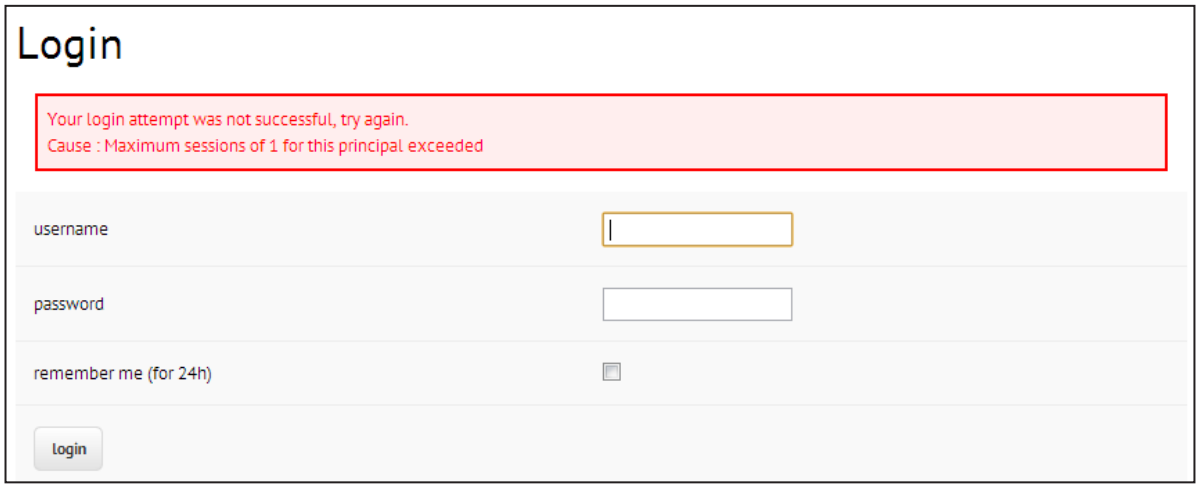


Figure 2: Error message in case of exceeding maximum number of simultaneous sessions

Logging in with the wrong username or password will generate a different error message (Figure 3). In case you forget your password, you can contact the S-Risk administrators, who will send you an e-mail with a new password.

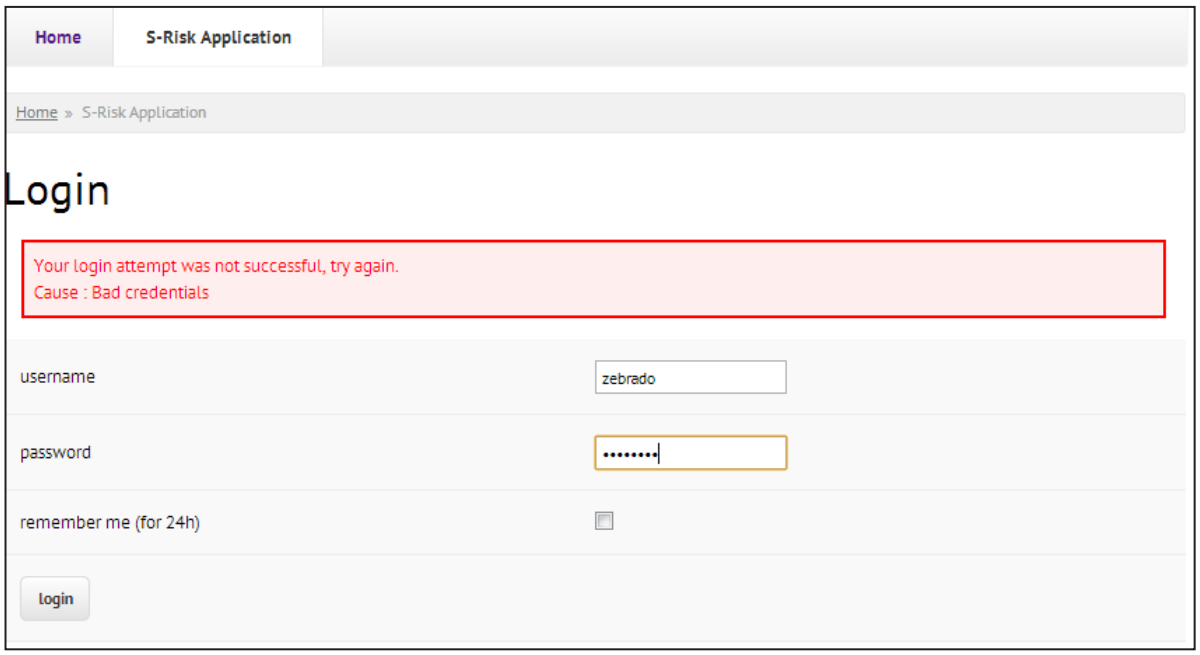


Figure 3: Error message in case of wrong username or password

Once you are logged in successfully, the S-Risk overview page will appear.

CHAPTER 3 MANAGING SIMULATIONS

3.1. THE OVERVIEW SCREEN

After logging in to the S-Risk web application, the S-Risk overview page will appear (Figure 4). At the top left, you can see for which region you are currently logged in (here: Flanders/Brussels). The user interface distinguishes 4 main panels:

1. Menu bar
2. Overview of existing simulations
3. Simulation summary
4. Simulation details

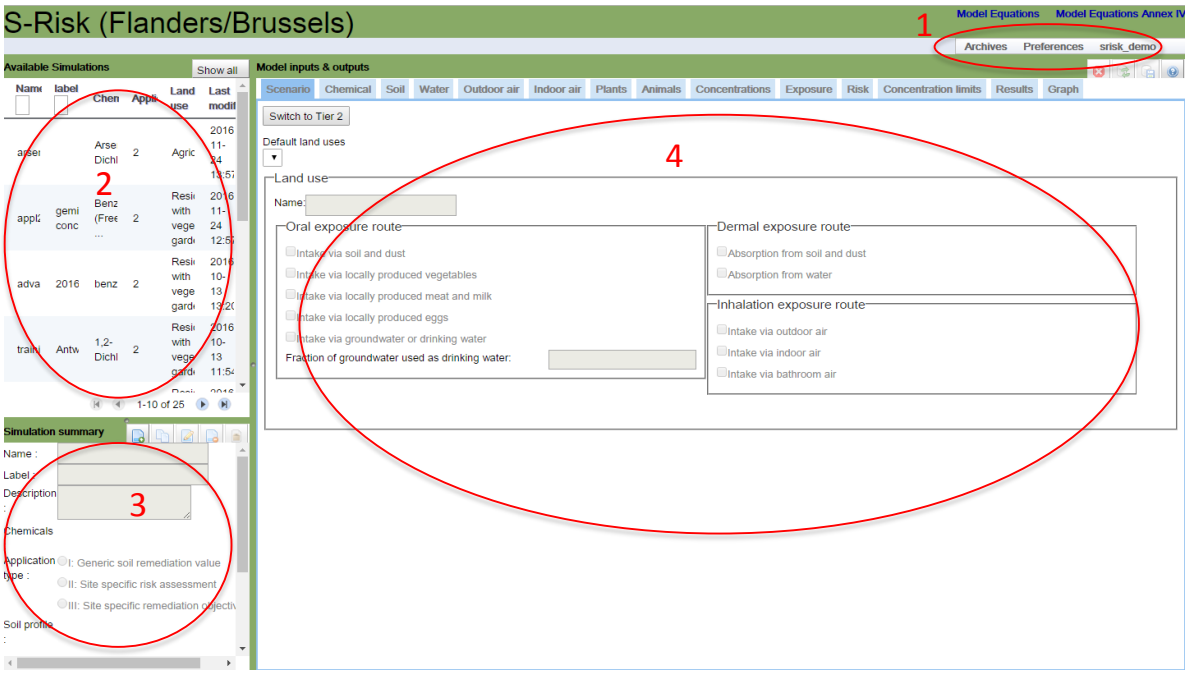


Figure 4: S-Risk user interface

The vertical border line between the left and right panels can be shifted horizontally to increase/decrease the size of the panels. Similarly, you can shift the horizontal border between the simulations overview table and the simulation summary panel.

3.1.1. MENU BAR

When you select your username in the menu bar, you can choose to change your password or to log out (Figure 5).

IMPORTANT: it is important to explicitly use the "Logout" command when you leave the web application, before you close the browser. If you forget this, you will have to wait for half an hour before you will be able to log in again.

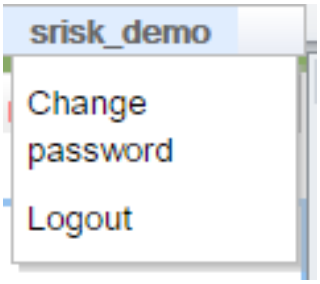


Figure 5: Account settings menu

When you choose the Preferences menu, you can select your language. The languages available are English and Dutch (Figure 6). When you change the language settings, the application will warn you that any unsaved data will be lost. Be sure to save your data before switching languages.

Figure 6: Preferences menu

When you press on "Archives", the Archive page on which you can find all your archived simulations will be opened (Figure 7). Analogously to the table with available simulations (see also 3.1.2), the "Name" and "Label" columns of this page also provide search fields directly below the column header. By typing a partial simulation/label name in this search field and pressing <Enter>, the simulations list will be filtered to only show the matching simulation names/projects. Simulations can also be filtered based on the archive date. The archived simulations can be sorted by "Name", "Label" and "Archived on" by clicking the respective column heading. When you press behind a certain simulation on the "Restore" button ( ), the simulation will be restored and will be available again in the table with available simulations of the S-Risk main screen. Returning to the S-Risk main screen is possible by clicking "Back" at the top right.

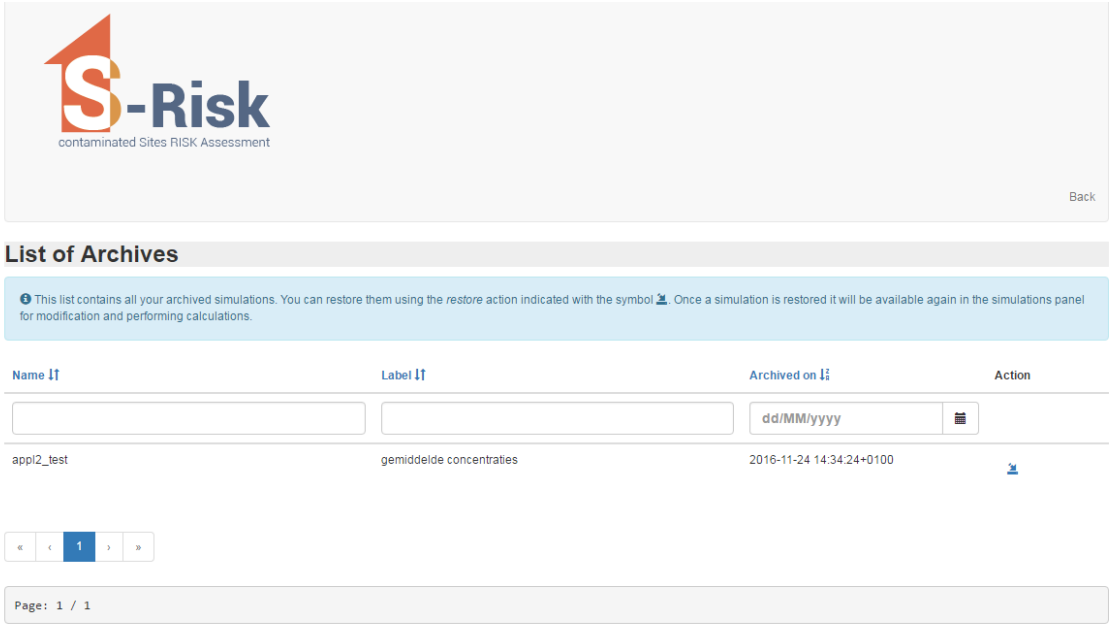


Figure 7: Archive page

3.1.2. OVERVIEW OF EXISTING SIMULATIONS

If you have already created simulations in the past, these will be visible in the list on the upper left side of the page (“Available simulations”, Figure 8). This list shows key identifying information of all simulations, to quickly find the simulation you need. If no simulations are present yet, the “Available simulations” list on the left will be empty.

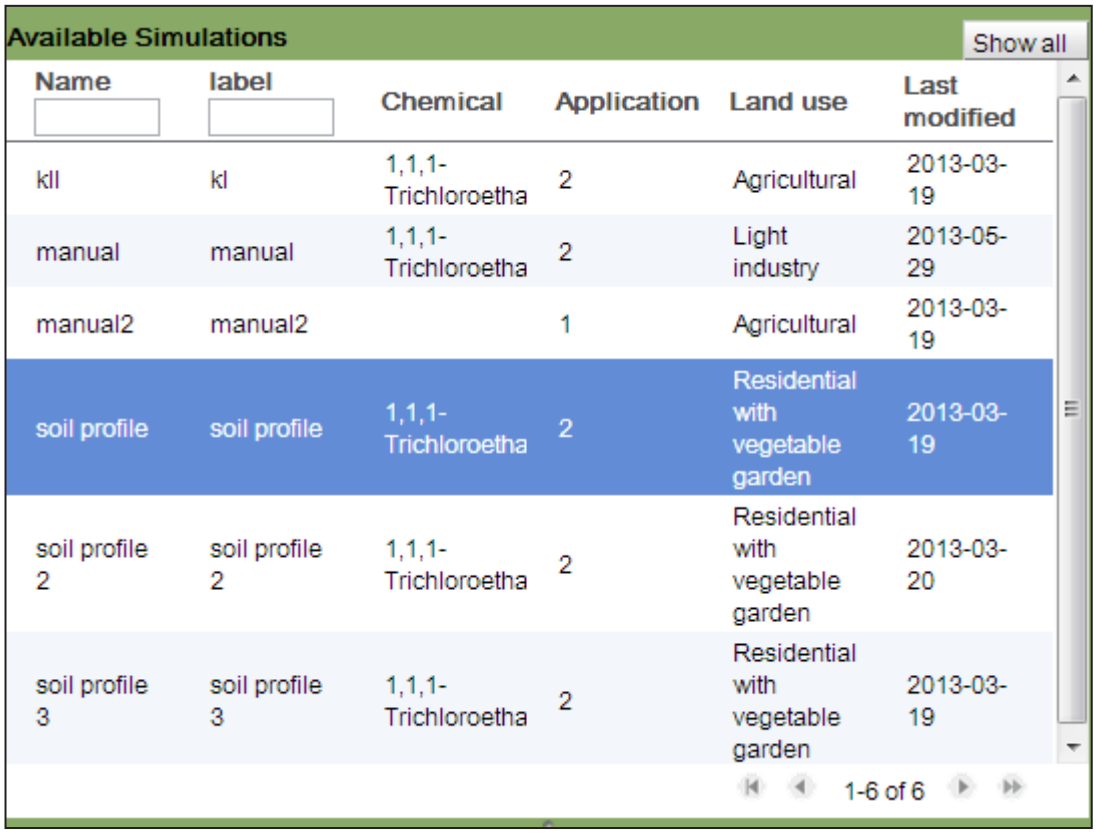


Figure 8: Overview of existing simulations

The "**Name**" and "**Label**" columns of this list also provide search fields directly below the column header. By typing a partial simulation/label name in this search field and pressing <Enter>, the simulations list will be filtered to only show the matching simulation names/projects. This way, simulations can be found easily when the number of simulations grows larger. Search results are presented in a page view once there are more than 10 results.

Simulations can be sorted by "Name", "Label" and "Last modified" by clicking the column heading.

On top of the simulation, there is a toggle button named "**Show all**". This toggle button can be used to view either your own simulations or all the simulations within your company for a certain region. You will be able to view simulations of your colleagues, but you will not be able to modify them.

Simulations have colour codings:

- Grey colour: no modifications possible (this is a simulation of a colleague or one of your own if you only have *read-only* access);
- Red colour: the most recent calculation failed (only visible for your own simulations);
- Yellow colour: calculations are running for your simulation;
- Blue colour: selected simulation (summary information is visible in the simulation summary panel).

3.1.3. SIMULATION SUMMARY

Summary information on the currently selected simulation will be displayed on the lower left. Depending on your browser, the summary information will show a graphical representation of the soil profile (as is the case in the screenshot in Figure 9) or will indicate that this feature is not supported (this is the case for older browsers, e.g., Internet Explorer 8 or lower do not support this). The absence of this overview graphic does not impact the S-Risk model calculations in any way.

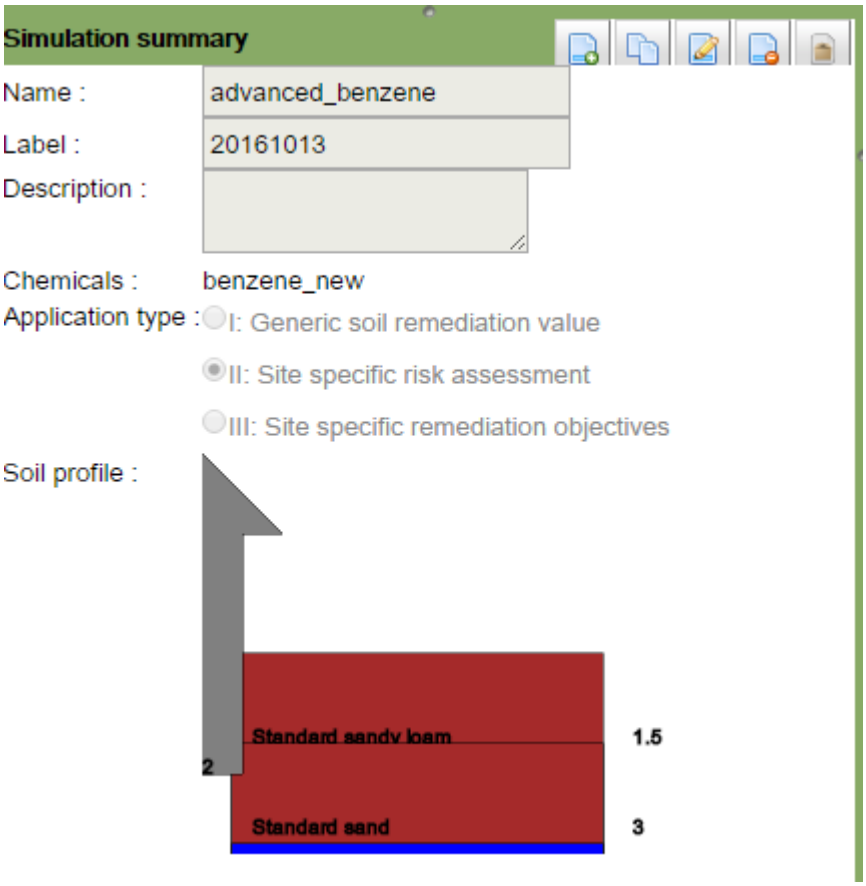


Figure 9: Simulation overview

Four actions can be performed on a selected simulation when you have *read-write* access:

- copy ( );
- edit ( );
- delete ( );
- archive ( ).

Evidently, you can also start a new simulation ( ) when you have *read-write* access. Information with regard to the requirements for a new simulation are given in *3.2 Starting a new simulation*. Further details for managing existing simulations are given in *3.3 Managing your simulations*.

3.1.4. MANAGING THE DATA DURING A SIMULATION

When entering or modifying data during the creation of a simulation, data entry can be managed from the menu at the top of the simulation details panel (Figure 10):

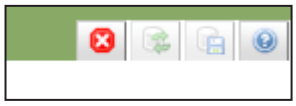


Figure 10: Menu for managing the data during a simulation

- "Reset defaults" button ( ): this button is relevant to the first three tabs and restores the selected land use, selected chemical or soil type parameters to the defaults they were derived from;
- "Cancel" button ( ): data changes since the last save action are canceled;
- "Save simulation" button ( ): data are saved to the S-Risk database;
- "Help" button ( ).

In addition to pressing the "Save simulation" button, data are also saved when you switch tabs. As soon as your data are saved to the S-Risk database, they can't get lost due to computer, browser or network failure. So, in the worst case, you can lose only the data you entered or were entering in the last open S-Risk tab.

3.2. STARTING A NEW SIMULATION

A new simulation can be started by clicking the "**Create new simulation**" button in the "Simulation summary" header (Figure 11). The "Simulation summary" fields will become active and the "**Name**", "**Label**" and "**Description**" of the simulation can be filled in (the "Name" field is mandatory).

It is up to the user to provide sensible names, labels and descriptions for the various simulations. The label field, for instance, can be used as an uniform identifier of simulations within a company.

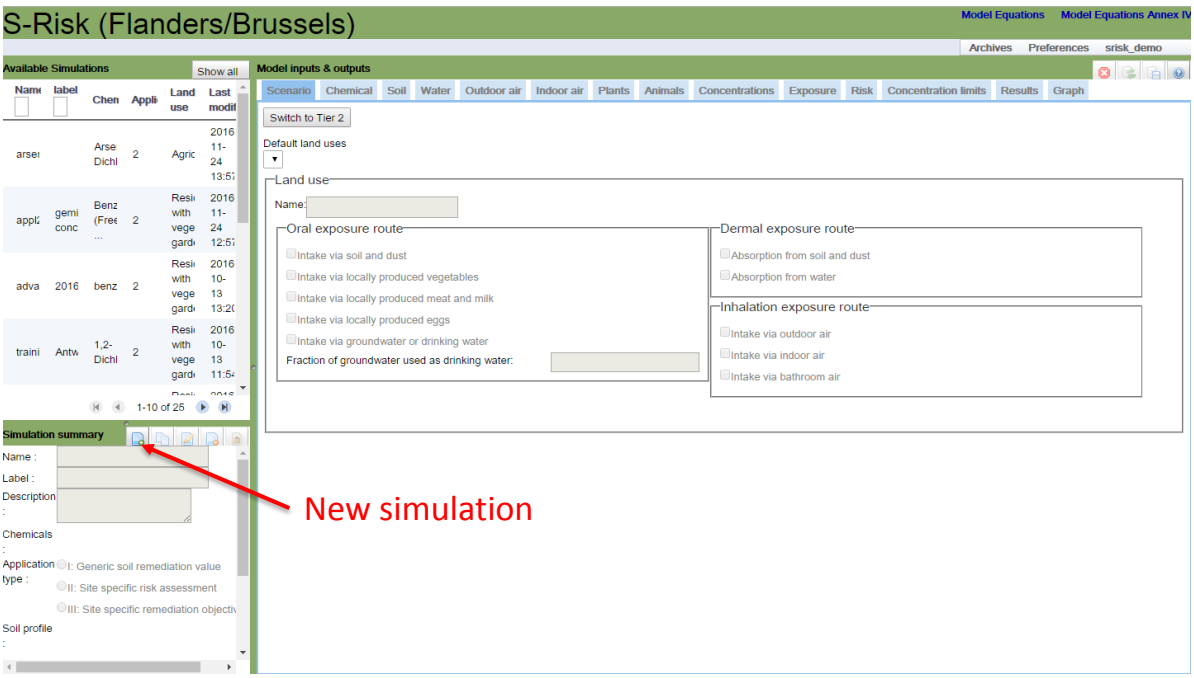


Figure 11: Starting a new simulation

Also, you need to indicate the application type for your simulation:

- Type I - generic soil remediation value: the model will calculate soil remediation values with default settings. You can choose land use type, soil type and chemical. You can only modify certain soil type parameters and chemical parameters, all other parameter will be kept at their defaults;
- Type II – site specific risk assessment: the full flexibility of the model is provided under this option. You can fill in site-specific information for a human health risk assessment. Human risks will be calculated starting from soil and/or groundwater concentration measurements (*forward* calculation);
- Type III – site specific remediation objectives: the full flexibility of the model is provided under this option and all site-specific information can be entered. The soil layer for which you want the remediation objective to be calculated should be specified in the *Concentrations* tab (*backward* calculation: we calculate soil concentrations corresponding to certain risk thresholds).

Simulations are created as application II by default. You can modify the application type by selecting application I or III.

NOTE: When switching from application type II or III to application type I, following changes will occur: only 1 soil layer will be retained (if no soil layer was created yet, a generic layer will be created), some settings are restored to their defaults (such as buffer length, calculation of leaching, …). Chemicals and land uses (even when customized) will be retained. It is therefore recommended not to switch from application II or III to I.

After specifying the name, label, description and application type, the simulation is created by clicking the "**Save**" button 

. After this, you can proceed to the "Model inputs and outputs" panel on the right, to specify or adjust the detailed model parameters. After creating the simulation, the *Scenario*, *Chemical* and *Soil* tabs will become available. The remaining tabs will become active once you have specified at least one chemical and a valid soil profile.

3.3. MANAGING YOUR SIMULATIONS

The available simulations are visible in the "Available simulations" panel on the upper left. You can select a simulation by simply clicking on it. This will allow you to manage the simulation with the buttons in the "Simulation summary" bar. Besides the "**Create new simulation**" button described above, four other buttons are visible:

"Copy selected simulation" 

This button allows you to copy or *clone* an existing simulation. You will need to specify a new simulation name (and label and description if appropriate) in the "Simulation summary" panel, after which a new simulation will be created with the same parameter values of the cloned simulation. If the application type is changed, parameter values can however be reset as explained above under the discussion of the application types.

"**Modify selected simulation**" 

You can modify the name, label and description, as well as the application type of the simulation that is currently selected in the "Available simulations" panel.

"Delete selected simulation" 

This button will delete the currently selected simulation. A confirmation screen will appear before the effective removal of the simulation will take place. **NOTE: the full configuration of the simulation will be removed from S-Risk, so be careful with this button.**

"Archive selected simulation" 

This button allows you to manually archive a selected simulation (simulations not consulted during the last two years will be archived automatically). A confirmation screen will appear before the simulation will be archived effectively.

3.4. MODIFYING MODEL PARAMETERS

Model parameters can be modified in the tabs on the "Model inputs & outputs" panel. If there is not enough space to show all tabs, little arrows will appear at the left side of the tabs (Figure 12).

Figure 12: Scrolling tabs

When you click the left arrow ( ) the tabs will move to the left. When you click the right arrow ( ) the tabs will move to the right.

The *default setting* of S-Risk is basic mode or Tier 1. Tier 1 provides access to a limited number of options and parameter values. Tier 1 should be sufficient for initial risk assessment and more routine simulations. Access to expert mode is available per tab via the "**Switch to Tier 2**" toggle button (Switch to Tier 2). Clicking this button will provide access to additional parameters or settings, either by showing them directly on the screen or by the appearance of an additional button. When you are in Tier 2, you can switch back to Tier 1 by clicking once again the toggle button "Switch to Tier 1" (Switch to Tier 1). Data that have been modified under Tier 2 will keep their customized values.

Some fields are provided with a text balloon ( ). Clicking this symbol, allows you to fill in comments for this field. For some fields, it is required to fill in a comment when the parameter value or setting is changed. In that case, the comment field will open automatically when the value is changed. If a field is provided with a comment, the text balloon will appear with a small pencil ( ).

3.5. ABOUT S-RISK VERSIONS AND SIMULATIONS

The S-Risk web application is continuously being worked on, and regularly new application updates are made available online. Each of these updates is uniquely identified with a version number, and can contain both changes to the model code (calculations) as to the default parameter values.

Consequently, for each simulation, there are 2 version numbers that are determining the end result:

- the version in which the simulation was created (determining the set of default parameter values used to initialize the simulation), and
- the version in which the simulation was last calculated (determining the actual model version used for calculations).

To keep this transparent and clear, every generated PDF or online report mentions both versions at the bottom of the page. This makes it easier for third parties to evaluate the simulation results, and get an immediate idea of which parameter values or model code were used.

Once a simulation is created, its parameter values will NOT be adjusted, not even when the S-Risk application itself is updated. For instance, when a simulation created in S-Risk 1.0.3 is simulated in S-Risk 1.0.10, the old default parameter values will be used as input for the 1.0.10 model calculations, unless they were adjusted by the user him/herself.

One important exception to this rule is the *buffer space* parameter. This is the minimum distance between contamination and building floor or walls that is considered when calculating volatilization of a compound from soil/groundwater to the indoor environment. This parameter is available in the indoor air tab of the S-Risk interface (at Tier 2)', and is also included in the extended report (not in the online report!):

- In application I, the buffer space is 0.75 m;
- In applications II & III, the buffer space is 0.10 m.

Although this parameter is visible and can be adjusted, altering its value would require a very solid justification. It is unlikely that any change in the bufferspace would be accepted in regular risk assessments[1].

IMPORTANT: in S-Risk versions before 1.0.10, the buffer space was set to 0.05 m for applications II and III.

When the application type for such "older", pre-1.0.10 simulations is changed, the buffer space parameter is adjusted too to the new value (0.10 m for applications II and III). If the application type is not changed for a pre-1.0.10 simulation, the old buffer space value remains unchanged (0.05 m for applications II and III), just as described earlier for the other parameters.

[1] Adjusting the buffer space can only be justified if a generic soil remediation value has been calculated with Application I (default buffer space 0.75 m). To evaluate the contribution of exposure routes and exposure pathways, an Application II simulation can then be run with the buffer space value adjusted to 0.75 m.

CHAPTER 4 APPLICATION II SIMULATIONS

Guidance with regard to the set-up of an application II simulation follows the order of the tabs as they appear on the S-Risk panel “Model inputs & outputs”. In case of a new simulation, only the Scenario, Chemical and Soil tab will be available for modification. Once these are filled in, the other tabs will become active. In case of the modification of an existing simulation, all tabs will be available once the simulation is selected, copied or edited.

4.1. SCENARIO TAB

4.1.1. TIER 1

A drop-down list is available to select the appropriate land use type for your simulation (Figure 13). Once selected, the land use box will show the associated exposure pathways grouped by exposure route.

The menu choices represent a number of *default* land use types, with fixed parameter values.

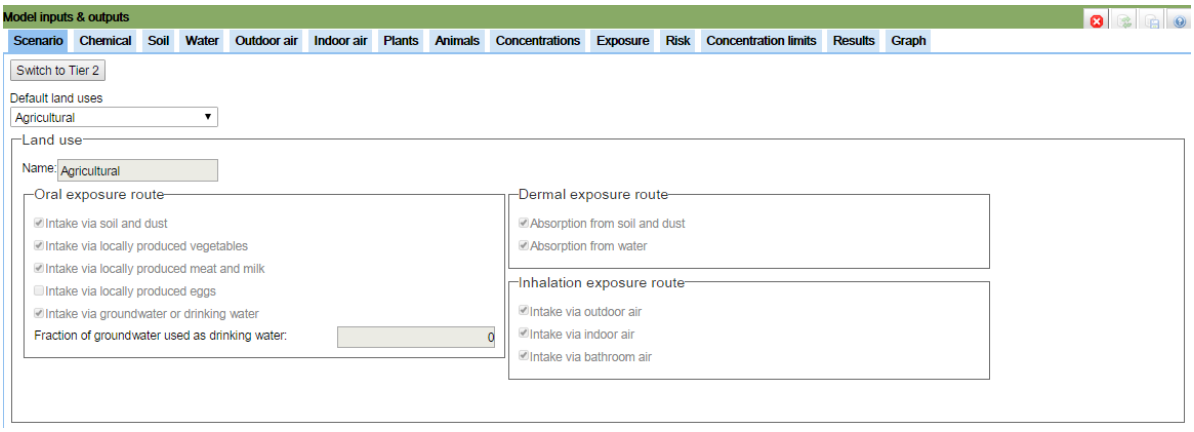


Figure 13: Scenario tab at Tier 1

Attention: When you change a land use type within your simulation, the following parameter values will be reset to their corresponding land use defaults:

- *Scenario* tab: time patterns on site, soil & dust ingestion rates, fraction of soil contributing to soil & dust ingestion and fraction of groundwater used as drinking water;
- *Water* tab: enter/calculate groundwater concentration and fraction of drinking water intake coming from site;
- *Outdoor air* tab: terrain roughness length;
- *Indoor air* tab: building type, state of floor, basic air exchange rate for indoor space and fraction of soil in indoor dust;
- *Exposure* tab: food consumption rates for vegetables & animal products and fraction of local origin for vegetables & animal products.

4.1.2. TIER 2

Under Tier 2, it is possible to modify the default land uses (Figure 14).

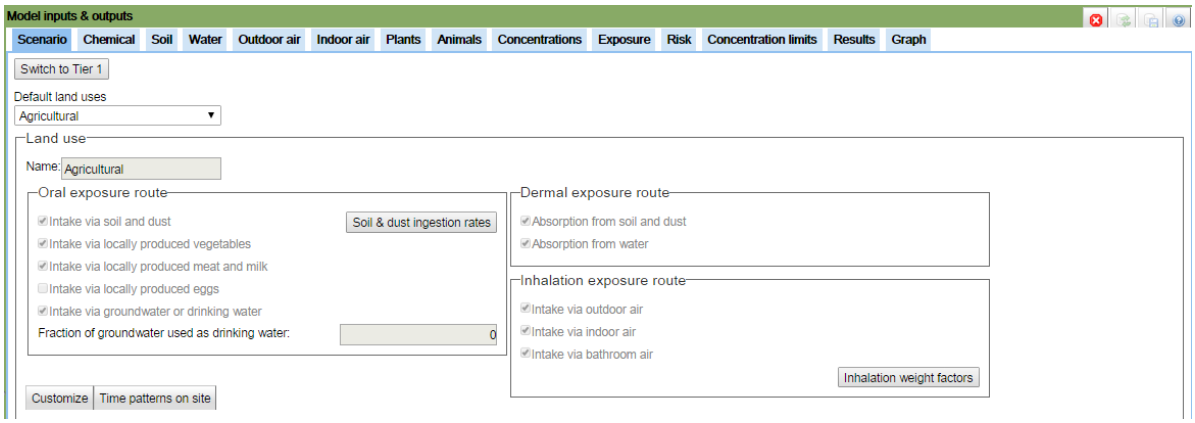


Figure 14: Scenario tab at Tier 2

In order to specify your own land use type, you can modify one of the default land use types by clicking the "**customize**" button. After entering a new name for the land use type, exposure pathways and parameter values will become available and editable.

Modification of the land use type can be done at two levels:

→ **Modifying the land use type by selecting exposure pathways**

The scenario tab shows the active exposure pathways as they were set for the default land use type. Exposure pathways can be toggled active and inactive by clicking the corresponding checkboxes before an exposure pathway.

Attention: Exposure pathways can now be toggled active and inactive without restriction. We recommend not to add exposure pathways that were not active in the default land use type you started from (except for intake via locally produced eggs), because this could lead to inconsistent results**.**

Some of the exposure pathways are linked, such that when de-activating/activating one of them will automatically impact the de-activation/activation of the other.

If a certain exposure pathway is deactivated, the associated parameters in the subsequent tabs become irrelevant. This will be indicated when the tabs are discussed.

→ **Modifying the land use type by modification of exposure factors**

Following exposure factors can be modified in the scenario tab for a customized land use.

Fraction of groundwater used as drinking water

By default, the fraction of groundwater used as drinking water for human consumption is set to 0. This can be modified by adding a fraction value between 0 and 1 in the "Fraction of groundwater used as drinking water" field. The calculations will then use a fraction-weighted concentration based on the groundwater and water supply concentrations.

Time patterns on site

The time spent on the site can be modified by clicking the "**Time patterns on site**" button. A table will appear (Figure 15).

Time patterns on site

	Sleep (h/d)	Awake inside (h/d)	Outside (h/d)	Total on site (h/d)	weekly exposure frequency (d/wk)	yearly exposure frequency (wk/y)
1-<3yrs	0	0	0	0	5	47
3-<6yrs	0	0	0	0	5	47
6-<10yrs	0	0	0	0	5	47
10-<15yrs	0	0	0	0	5	47
15-<21yrs	0	7	1	8	5	47
21-<31yrs	0	7	1	8	5	47
31-<41yrs	0	7	1	8	5	47
41-<51yrs	0	7	1	8	5	47
51-<61yrs	0	7	1	8	5	47
>=61yrs	0	7	1	8	5	47

OK Cancel

Figure 15: Time pattern table

Following parameters can be modified:

- Time sleeping;
- Time awake inside;
- Time outside;
- Exposure frequency in days per week;
- Exposure frequency in weeks per year.

Soil and dust ingestion rates

Soil and dust ingestion rates are age and activity dependent, and can be modified by clicking the "**Soil & dust ingestion rates**" button. In case of scenarios with *continuous exposures* (agricultural,

residential, industrial and for region Flanders/Brussels also holiday resort), a table will appear showing a daily ingestion rate (IR) of soil and dust, and a fraction of soil in ingestion (Figure 16). The fraction of soil in ingestion distributes the total ingestion rate over outside soil and inside settled dust. The distribution over soil and settled dust is therefore independent of the time spent outside/inside. In case of scenarios with *intermittent exposures* (day recreation), a table will appear showing hourly soil ingestion, and hourly dust ingestion rates (Figure 17). The ingestion of outdoor soil and of indoor settled dust on a daily basis is therefore dependent upon the time spent outside/inside.

We recommend not to change these values.

Ingestion Rates

	IR soil/dust daily (mg/d)	Fraction soil
1-<3yrs	0,0E0	0,0E0
3-<6yrs	0,0E0	0,0E0
6-<10yrs	0,0E0	0,0E0
10-<15yrs	0,0E0	0,0E0
15-<21yrs	2,6E1	2,0E-1
21-<31yrs	2,6E1	2,0E-1
31-<41yrs	2,6E1	2,0E-1
41-<51yrs	2,6E1	2,0E-1
51-<61yrs	2,6E1	2,0E-1
>=61yrs	2,6E1	2,0E-1

OK Cancel

Figure 16: Ingestion rates table for land uses with continuous exposure

Ingestion Rates

	IR soil hourly (mg/h)	IR dust hourly (mg/h)
1-<3yrs	2,6E1	4,0E0
3-<6yrs	2,0E1	3,0E0
6-<10yrs	1,3E1	2,0E0
10-<15yrs	1,1E1	2,0E0
15-<21yrs	9,0E0	2,0E0
21-<31yrs	5,0E0	1,8E0
31-<41yrs	5,0E0	1,8E0
41-<51yrs	5,0E0	1,8E0
51-<61yrs	5,0E0	1,8E0
>=61yrs	5,0E0	1,8E0

OK Cancel

Figure 17: Ingestion rates table for land uses with intermittent exposure

Inhalation weight factors

Inhalation exposure and corresponding risk are calculated as time-weighted concentrations. To account for differences in inhalation rate by activity, inhalation weight factors are used. These can be modified by clicking the "**Inhalation weight factors**" button (Figure 18). The weight factors express the ratio of the inhalation rate at the activity level compared to the inhalation rate at normal activity (i.e., inhalation rates for residential scenarios). The influence of age on inhalation is taken into account in a different weight factor present under the Exposure tab.

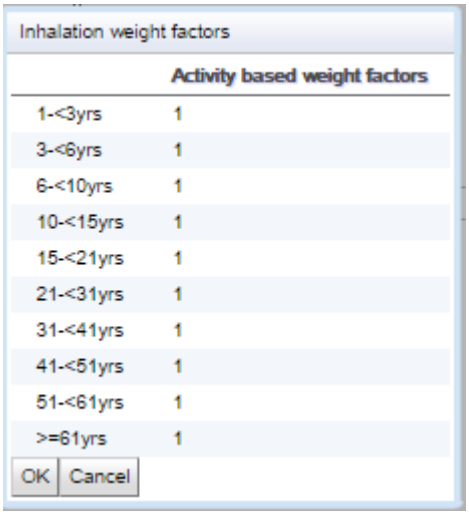


Figure 18: Activity based weight factors for inhalation

4.2. CHEMICAL TAB

The *Chemical* tab allows to:

a) add one of the default built-in chemicals from the drop-down list to the simulation;

b) customize a built-in chemical (Tier 2);

c) add a new chemical (Tier 2).

4.2.1. ADDING DEFAULT CHEMICALS

A database of built-in chemicals is provided with S-Risk. This list contains the chemicals for which soil remediation values are available, as well as a limited number of other chemicals that have been part of documents in preparation of soil remediation values (e.g., chromium VI, organic and elemental mercury and total petroleum hydrocarbon fractions).

Chemical substances can be added using the drop-down menu and clicking the "**Add**" button (Figure 19). More than one chemical can be selected by repeatedly selecting a chemical and clicking the "**Add**" button. The full list of added chemicals will be shown in the list on top of the tab. Chemicals can be removed from the simulation by selecting the chemical in the list and clicking the "**Delete**" button at the bottom of the tab.

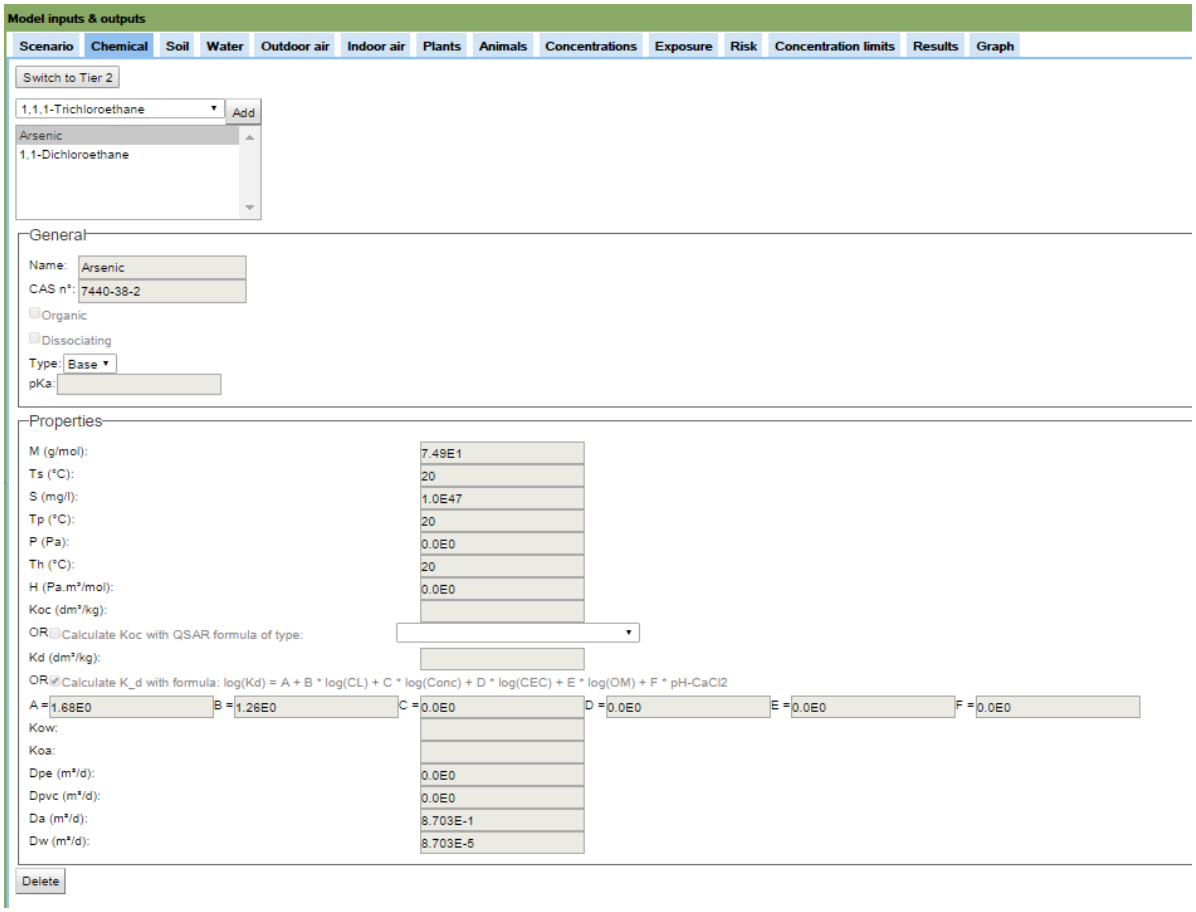


Figure 19: Chemicals tab at Tier 1

4.2.2. MODIFYING A CHEMICAL (TIER 2)

Added chemicals can be customized at Tier 2 by selecting them and clicking the "**Customize**" button at the bottom of the tab. After providing a new name for the chemical, the input fields for the chemical parameters will become active and can be modified. Customizing a chemical in the chemical tab will also give access to chemical related parameters in the Plants, Animals, Concentrations, Exposure, Risk and Concentration limits tabs. Also here, chemical dependent parameter values can be modified if necessary.

Attention: The chemicals copper, lead, nickel, mercury and zinc have special rules with regard to plant uptake relations and/or animal transfer factors. These rules can be found in the chemical-specific documentation (substance data sheets). To avoid confusion with regard to the models used, these chemicals can NOT be modified or customized. If you would like to work with modified versions of these chemicals, you will need to configure them starting from the "(Blank chemical)" template.

Details with regard to each of the fields in the chemical tab are given under Adding a new chemical.

4.2.3. ADDING A NEW CHEMICAL

If you want to add a new chemical, you can select the "(Blank chemical)" from the bottom of the drop-down menu and add it to the simulation using the "**Add**" button. This can be done under Tier 1. The chemical tab will show empty fields for this blank chemical. To fill in these fields, you need to go to Tier 2 and customize the chemical as specified under Modifying a chemical.

- **CAS n°:** optional field
- **Organic**: by default, the blank chemical type is inorganic, for organic chemicals you should select the "organic" check box
- **M** - molecular mass

Parameters requirements differ by type of chemical (inorganic, organic):

→ **Data requirements specific for inorganic chemicals**

Parameter	Information
S - solubility in water at temperature **T_s** **P** - vapour pressure at temperature **T_p**	• required • for inorganic chemicals, the solubility is generally set at a very high value (e.g., 1.10^5 mg/l). The model automatically limits the calculated soil pore water concentration to the solubility. In case of a low solubility, this would overrule the K_d concept for inorganic chemicals.
H – Henry's law coefficient at **T_h**	• required • This value will generally be 0, except for volatile inorganic chemicals.
K_d – sorption coefficient soil/water	• required • a soil sorption coefficient can be filled in as a single value or as a relationship between the $\log_{10}$ of the K_d and soil properties (and total concentration in soil). In the latter case, intercept and slopes with regard to clay concent (**CL** in %), total soil concentration (**Conc** in mg/kg dm), cation exchange capacity (**CEC** in meq/100 g), organic matter content (**OM** in %) and **pH** (measured in $CaCl_2$ solution) can be filled in.
D_pe – permeation coefficient through polyethylene **D_pvc** – permeation coefficient through PVC	• these values are used to calculate the permeation (diffusion) through supply water pipes. • for inorganic chemicals, the values will generally be zero.
D_a – diffusion coefficient in air	• these values are used to calculate diffusion parameters related to evaporation to ambient air and vapour intrusion into

D_w – diffusion coefficient in water	buildings. • in case of non-volatile inorganic chemicals, these parameters are irrelevant. In case of volatile inorganic chemicals, the parameters can be filled in or calculated from molecular mass.

→ **Data requirements specific for organic chemicals**

If an organic chemical is to be added, the checkbox "**organic**" should be activated. If the chemical has dissociating properties, the checkbox "**dissociating**" should be activated. In the latter case, you have to choose between **acid** or **base** dissociation from the drop-down list and fill in a pKa (acid dissociation constant). For dissociating chemicals, the K_d is calculated by the model using a built-in algorithm. No K_{oc} is required then.

If – for a dissociating chemical – a K_{oc} value is available at the appropriate soil pH, you can also choose not to activate the option "dissociating" and fill in the available K_{oc} value. This is only allowed for calculations within the pH range of the K_{oc} value.

Parameter	Information
S - solubility in water at temperature **T_s** **P** - vapour pressure at temperature **T_p**	• <u>required</u> • it is recommended to fill in solubility and vapour pressure values for the same temperature and as close as possible to soil or ambient temperature. This is merely important if no value for the Henry-coefficient is filled in.
H – Henry's law coefficient at **T_h**	• optional • if a value for H is filled in, the associated temperature should be filled in as well. • if no value for H is filled in, the model will calculate it from vapour pressure P and solubility S, using the temperature of the vapour pressure. • the model will recalculate the value for H for the temperatures required in the model (soil temperature, shower water temperature).
K_oc – sorption coefficient organic carbon/water	• optional • if no Koc value is filled in, you have to activate the checkbox for calculation of the K_{oc} with a QSAR. You have to select the QSAR from the drop-down list.
K_ow – distribution coefficient octanol/water	• <u>required</u> • K_{ow} is used to calculate K_{oc} with QSARs , plant and animal transfer factors, and the

Parameter	Information
	dermal permeability coefficient (if the calculation option is chosen for the parameters).
K_oa – distribution coefficient octanol/air	• Optional • If no value is filled in, K_{oa} is calculated from K_{ow} and the Henry's law coefficient. • K_{oa} is used in plant transfer calculations.
D_pe – permeation coefficient through polyethylene **D_pvc** – permeation coefficient through PVC	• D_pe: Required • these values are used to calculate the permeation (diffusion) through supply water pipes.
D_a – diffusion coefficient in air **D_w** – diffusion coefficient in water	• optional • these values are used to calculate diffusion parameters related to evaporation to ambient air and vapour intrusion into buildings. • if no value is filled in, the values are calculated from molecular mass

4.3. SOIL TAB

The soil tab allows you to:

(a) define the soil profile, and

(b) specify the properties for the unsaturated soil layers.

When accessing the *Soil* tab for a new simulation, a default soil profile consisting of a single unsaturated layer and a groundwater table at 3 m depth will be visible (defaults of application I), as shown in Figure 20 for Tier 1 and in Figure 21 for Tier 2. When accessing the *Soil* tab under an existing simulation, the soil profile entered will be visible.

Selecting a soil layer by clicking on it shows the parameters of that soil layer.

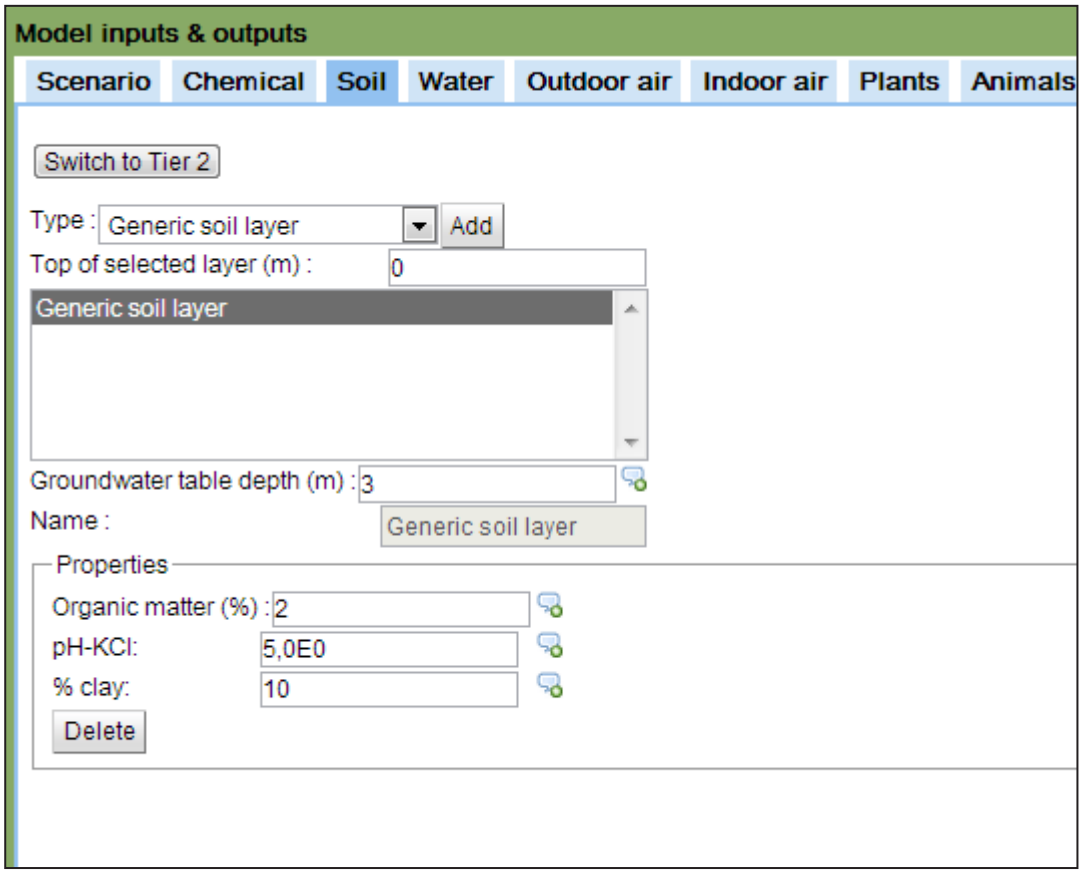


Figure 20: Soil tab at Tier 1

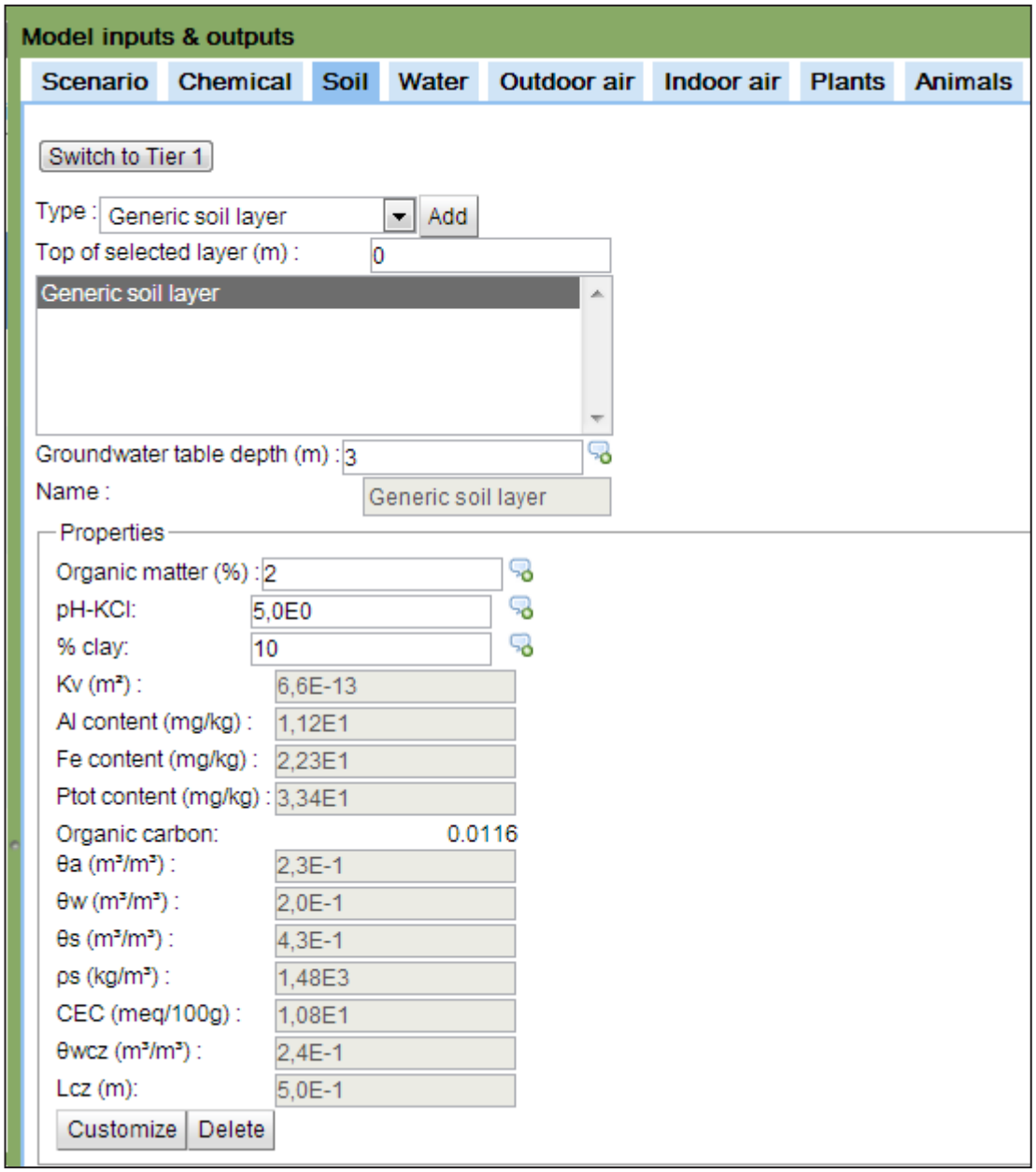


Figure 21: Soil tab at Tier 2

4.3.1. BUILDING THE SOIL PROFILE

The soil profile is built up layer by layer, by first selecting the appropriate soil type from the drop-down list next to the "**Type**" label and clicking the "**Add**" button.

Attention: When you generate a new soil profile, you first need to delete the default "generic soil layer" by selecting it and clicking the "**delete"** button at the bottom of the tab. Then you can select the appropriate soil type for the first soil layer from the drop-down list and add it to the soil profile.

There are two ways to build the soil profile:

1. The first option is to start with adding all layers of the soil profile by selecting the appropriate soil type and clicking the "**Add**" button. This is repeated for each layer in the soil profile. All added layers will appear in the list of added layers. The first layer added will appear with a depth of 0 m. The subsequently added layers will have a depth that shows an increase of 0.1 m with regard to the previous one. This way, the layers appear in the order you entered them. After addition of all layers, you can modify the depth according to the real profile, by selecting the layer and modifying the depth in the field "**Top of selected layer**";
2. The second option is to add each layer and immediately enter the depth according to your soil profile. The layer that is added first, will have a depth of 0 m assigned by the model. Each subsequently added layer will have a depth of 0.1 m and is selected so that you can access the field "**Top of selected layer**" and enter the appropriate depth. By following this option, it is possible that the last added layer does not appear in the profile on the correct depth (as it will have a depth of 0.1 m). Once you entered the correct depth, the layer will be shifted to its correct place in the profile.

Attention: The depth of the groundwater table should be below the sum of the depth of the building (slab, basement or crawl space floor) and the length of the buffer space. If conflicts occur, you have to leave the default soil profile, go to the indoor air tab and specify the building settings for vapour intrusion, including the depth of the building (slab, basement or crawl space floor). Switch then again to the Soil tab and enter the soil profile as required. The condition for groundwater depth in relation to building depth and buffer space results from the indoor air equations. These do not allow the calculation of vapour intrusion when the bottom of the basement is under groundwater level.

Once saved (either by clicking the Save button or by switching tabs), a graphical representation of the soil profile will appear in the "**Simulation summary**" panel on the left (under the condition that your web browser supports HTML5 canvas).

A soil layer can be removed from the profile by selecting it and clicking the "**Delete**" button at the bottom of the tab.

In the *Concentrations* tab you will be asked to fill in a concentration for each layer specified in the soil profile. The soil profile should therefore take into account changes in soil properties with depth, and the depth at which the concentrations were measured. For example: if an uniform soil profile with regard to soil properties exists, but concentrations were measured at two depths within that soil profile, two separate layers (with the same properties) should be created in the soil profile. This will enable to fill in the concentrations at the appropriate depth in the concentrations tab.

4.3.2. MODIFYING SOIL PROPERTIES

→ **Modifying soil properties at Tier 1**

At Tier 1, three soil properties can be modified by selecting the field and modifying the value (Figure 20): organic matter, pH-KCl and clay content. Although these parameters have default values in the database, they are considered as required, site-specific information.

Parameter	Information

Parameter	Information
organic matter	• Required, site-specific • The **organic carbon** content is automatically calculated from the organic matter content. • Used for calculation of distribution in soil.
pH_KCl	• Required, site-specific • Soil pH should be filled in as a pH-KCl measurement; the model automatically converts the value to pH-$CaCl_2$ (inorganic chemicals) or pH-H_2O (dissociating organic chemicals). • Parameter only important for inorganic chemicals if the K_d relation and/or BCF relation has a slope for pH-$CaCl_2$, and for organic dissociating chemicals.
% clay	• Required, site-specific • Should be consistent with the soil type chosen (due to its impact on choice of other soil properties). • Used for K_d/BCF calculations of inorganic chemicals if the relation has a slope factor for clay content.

When soil properties deviate significantly from the values in the default database, it is recommended to switch to Tier 2.

→ **Modifying soil properties at Tier 2**

Additional soil properties can be modified at Tier 2 by selecting the appropriate layer and clicking the "**Customize**" button at the bottom of the tab (Figure 21). First, you should rename the soil type for the layer by typing a name in the "N**ame**" field.

Parameters at Tier 2 require site-specific information that is not always available. The values can be measured or estimated. The appendix of the technical guidance document of S-Risk version Flanders/Brussels provides some information on how these parameters could be estimated from more readily available soil information.

Parameter	information
K_v – soil air permeability	• Default values for the soil type can be used. • Technical guidance document provides information on how to calculate values. • Important for vapour intrusion

Parameter	information
	calculations.
Al content	• Used for BCF (plant uptake) calculations of inorganic chemicals if a slope is filled in at the BCF relation (plant tab). • If so, then a site-specific value should be used.
Fe content	• Used for BCF (plant uptake) calculations of inorganic chemicals if a slope is filled in at the BCF relation (plant tab) (arsenic in chemical database). • Refers to reactive Fe (determined by oxalate extraction). • If relevant, a site-specific value should be used.
P_tot content	• Used for BCF (plant uptake) calculations of inorganic chemicals if a slope is filled in at the BCF relation (plant tab) (arsenic in chemical database). • If so, then a site-specific value should be used.
θ_a – volumetric air content **θ_w** – volumetric water content **θ_s** – soil porosity	• It is recommended to modify these values if soil type parameters as clay content are modified. • Information to calculate values is given in the technical guidance document.
ρ_s – soil bulk density	• Information to calculate values is given in the technical guidance document.
CEC – cation exchange capacity	• Parameter only important for inorganic chemicals if the K_d relation has a slope factor for CEC. • If so, site-specific information should be used.
θ_wcz – water content in the capillary zone	• Most relevant for the layer above the groundwater table. • Information to calculate values is given in the technical guidance document.
L_cz – thickness of the capillary zone	• Most relevant for the layer above the groundwater table. • Information to calculate values is given in the technical guidance document.

4.4. WATER TAB

The water tab (Figure 22) allows you to:

(a) specify whether a concentration in groundwater should be calculated from the unsaturated soil profile, or a measured concentration will be entered in the Concentrations tab,

(b) fill in parameter values for the calculation of the groundwater concentration,

(c) fill in the parameters with regard to the permeation of substances through supply water pipes, and

(d) specify drinking water exposure parameters.

The "permeation through supply water pipe" panel is only relevant if the exposure pathway "intake via groundwater or drinking-water" is active.

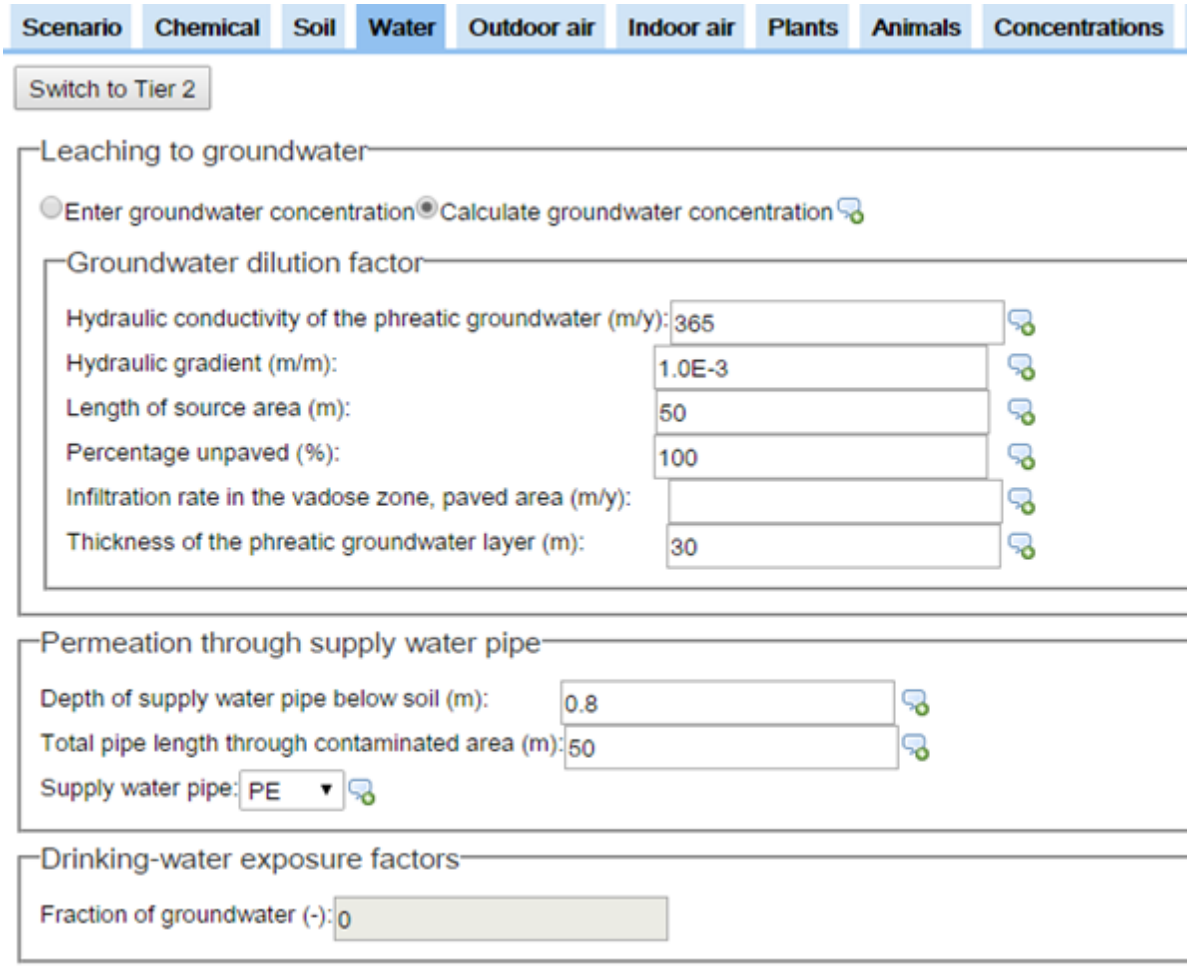


Figure 22: Water tab at Tier 1

4.4.1. LEACHING TO GROUNDWATER

When entering a new simulation, the "Calculate groundwater concentration" is activated by default. When a groundwater concentration is available for use in the calculations, you should select the "**Enter groundwater concentration**" option. You will be able to fill in the groundwater concentration in the Concentrations tab.

If you prefer to have the groundwater concentration calculated from the unsaturated soil profile by S-Risk, you should select the "**Calculate groundwater concentration**" option. The fields in the "dilution factors for groundwater" box will be available then at Tier 1 and Tier 2. The groundwater concentration due to leaching from the unsaturated zone is calculated according to a steady-state mass-balance model, similar to the F-Leach Tier 1 approach. Default values are consistent with the F-Leach parameterization. Guidance on choices for the site-specific parameters (except for length of the source area) can be found in the documentation of the F-Leach model on the OVAM website (http://www.ovam.be/jahia/Jahia/pid/1652). The concentration in groundwater due to leaching will be calculated for each specified soil layer under the Soil tab. Finally, the maximum value will be taken forward to the exposure calculations.

Parameter	Information
hydraulic conductivity	• Site-specific
hydraulic gradient	• Site-specific
length of source area	• Site-specific
percentage unpaved	• By default this value is set at 100 % • Could be lowered to represent site-specific conditions • If percentage unpaved is less than 100 %, a value for the infiltration rate for the paved area should be specified
infiltration rate in the vadose zone, unpaved area	• Default value, recommended not to modify
infiltration rate in the vadose zone, paved area	• Value should be filled in if the fraction unpaved is less than 100 %
thickness of the phreatic groundwater layer	• Site-specific

4.4.2. PERMEATION THROUGH SUPPLY WATER PIPE

→ **Tier 1**

If exposure to drinking-water is an exposure pathway in the scenario and when organic substances are added to the simulation, the fields for "permeation through supply water pipe" will be active. At Tier 1, three parameters should be specified: the depth of the supply water pipe below soil surface, the length of the supply water pipe through the contaminated area and the supply water pipe material. Permeation will be calculated if the pipe material is **polyethylene (PE) or PVC**. If the

material is "other", permeation is considered to be zero and the choice of any of the other parameter values is irrelevant.

Parameter	Information
depth of supply water pipe	• Site-specific • Will link automatically to the concentration in the corresponding soil layer except if a specific soil concentration for permeation is filled in later on (in the latter case only soil properties will be taken from the corresponding layer).
total pipe length through contaminated area	• Site-specific • If the representative concentration for supply water pipe deviates from the concentration in the soil profile, a specific value can be filled in at the Concentrations tab.
supply water pipe material	• Site-specific • Choice between PE, PVC or other. • If PE or PVC, permeation will be calculated using the permeation coefficient; if other, then permeation will be zero.

→ **Tier 2**

At Tier 2, three additional parameters become editable. They should only be modified if site-specific information is available.

Parameter	Information
internal radius of the supply-water pipe	• Default value, may be modified.
thickness of the wall of the supply-water pipe	• Default value, may be modified.
daily supply-water use	• Default, may be modified. • Default corresponds to average water use for a residence.

4.4.3. DRINKING WATER EXPOSURE FACTORS

The drinking-water exposure factors can only be modified at Tier 2.

Parameter	Information
fraction of groundwater used as drinking water	• Cannot be modified here, can be modified in the Scenario tab.

Parameter	Information
fraction of water consumption coming from site	• Land-use specific default • Can vary between 0 and 1 and relates to the fraction of total drinking water consumption of an individual that is from site water; the fraction is set < 1 if e.g., time spent on-site is much less than in residential situations (cfr. Industrial land use). • May be modified for specific land uses.

Drinking water consumption can be modified at Tier 2 by clicking the "**Water consumption rates**" button. Age-specific values are shown (Figure 23). It is recommended not to change these values without good justification.

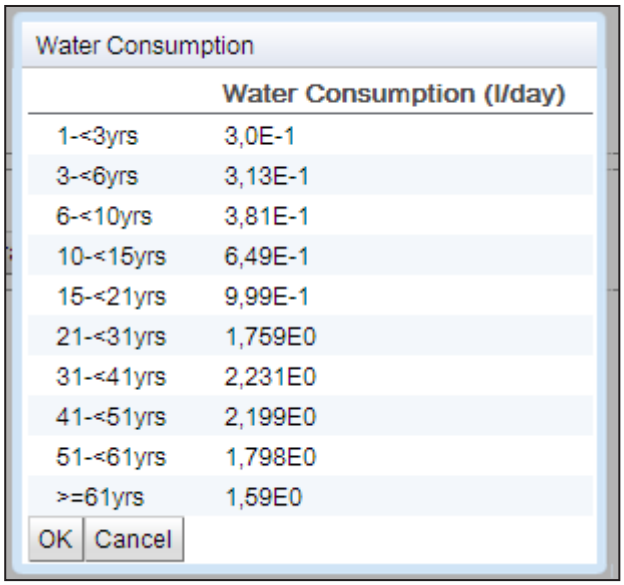


Figure 23: Water consumption table editable at Tier 2

4.5. OUTDOOR AIR TAB

Detailed information with regard to outdoor air should be looked at if there is potential outdoor air exposure, either due to volatilization or to soil resuspension. Soil resuspension should also be looked in view of the indoor inhalation exposure pathway through suspended particles. The *Outdoor air* tab (Figure 24) allows to specify a number of parameters for:

a) dilution in ambient air, and
b) soil resuspension.

Concentrations in outdoor air due to volatilization are calculated for each specified soil layer and for the groundwater layer. The soil concentration for each layer is assigned to the top of that layer to calculate the diffusion to the soil surface (except for the top layer). Dilution in ambient air is calculated using a box model. In a final step, the highest resulting outdoor air concentration due to

volatilization is selected and, after summation with the concentration resulting from soil resuspension, taken forward to the exposure calculations.

The concentration as a result of soil resuspension is added to the concentration due to volatilization, to calculate a final *overall* air concentration.

At Tier 1, only the length of the site (i.e., of the plume/contamination) in the dominant wind direction can be modified. At Tier 2 some additional parameters become editable.

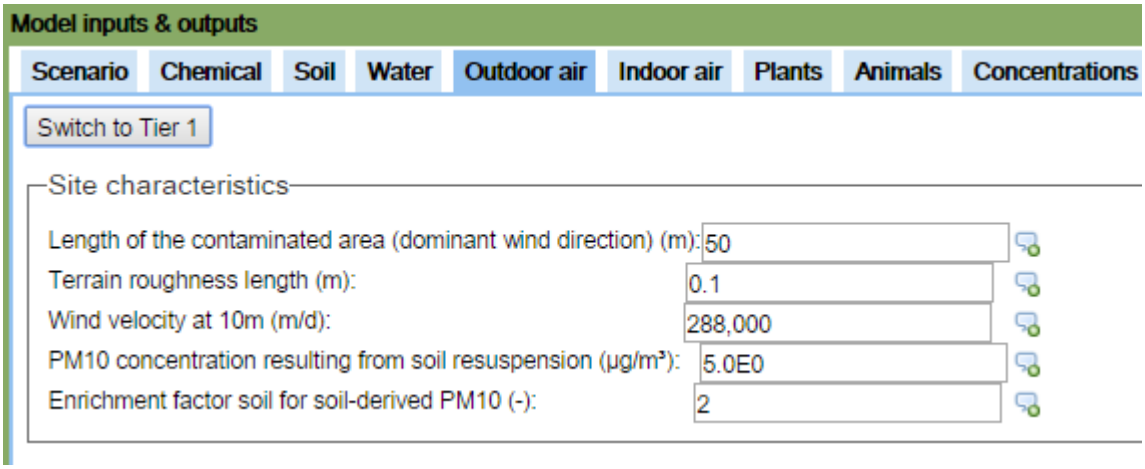


Figure 24: Outdoor air tab at Tier 2

Parameter	Information
length of the contaminated area in the dominant wind direction	• required (also visible at Tier 1) • Site-specific
terrain roughness length	• Default values, may be modified. • Values are land use specific. • Values as a function of land use and land coverage can be found in the technical guidance document.
wind velocity at 10 m	• Default value, recommended not to modify, depends upon geographical location. • Equation to calculate wind velocity as a function of geographical coordinate can be found in the technical guidance document.
PM_{10} concentration resulting from soil	• Default value, recommended not to modify.
enrichment factor soil soil-derived PM_{10}	• Default, recommended not to modify except if site-specific information is available. • Ratio between concentration on soil-derived PM_{10} and total soil concentration.

4.6. INDOOR AIR TAB

Detailing information in the indoor air tab is only relevant when a building is present or is simulated and indoor exposure can take place. Bathroom air parameters are only relevant when the exposure pathway bathing or showering is active. The indoor air tab allows you to specify the settings for:

a) vapour intrusion into buildings,
b) indoor settled dust,
c) indoor PM_{10}, and
d) bathroom air.

At Tier 1, a limited set of parameters related to vapour intrusion is accessible (Figure 25).

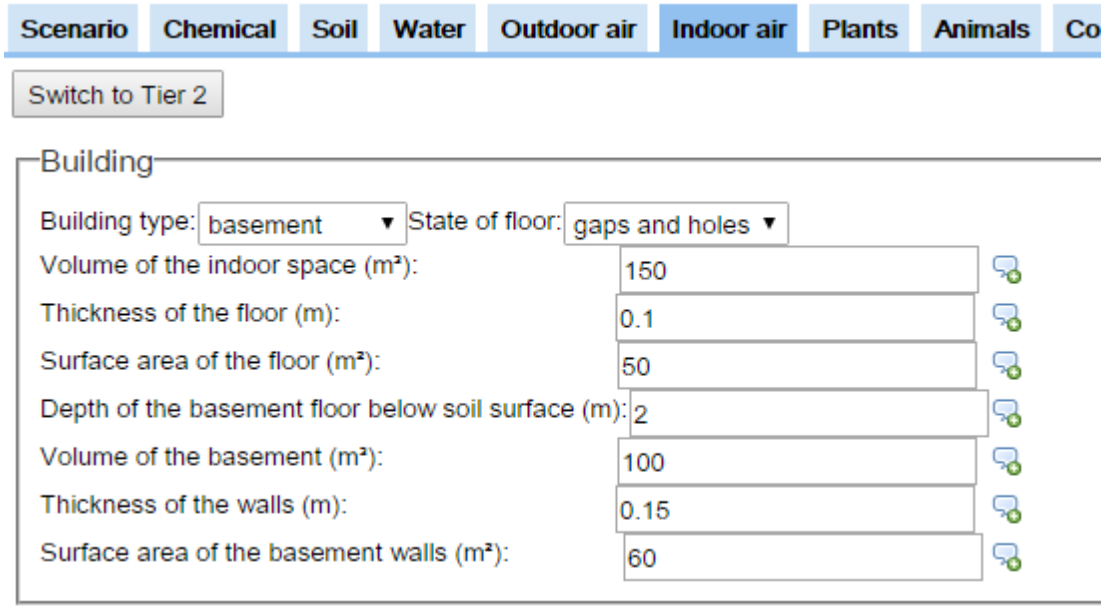


Figure 25: Indoor air tab at Tier 1

At Tier 2, some more parameters related to vapour intrusion become editable. In addition, the parameter related to the prediction of the indoor settled dust concentration, the concentration on indoor soil-related PM_{10} and the bathroom air concentration due to evaporation during showering become editable (Figure 26). In addition, a button "**Time patterns bathing and showering**" will become visible.

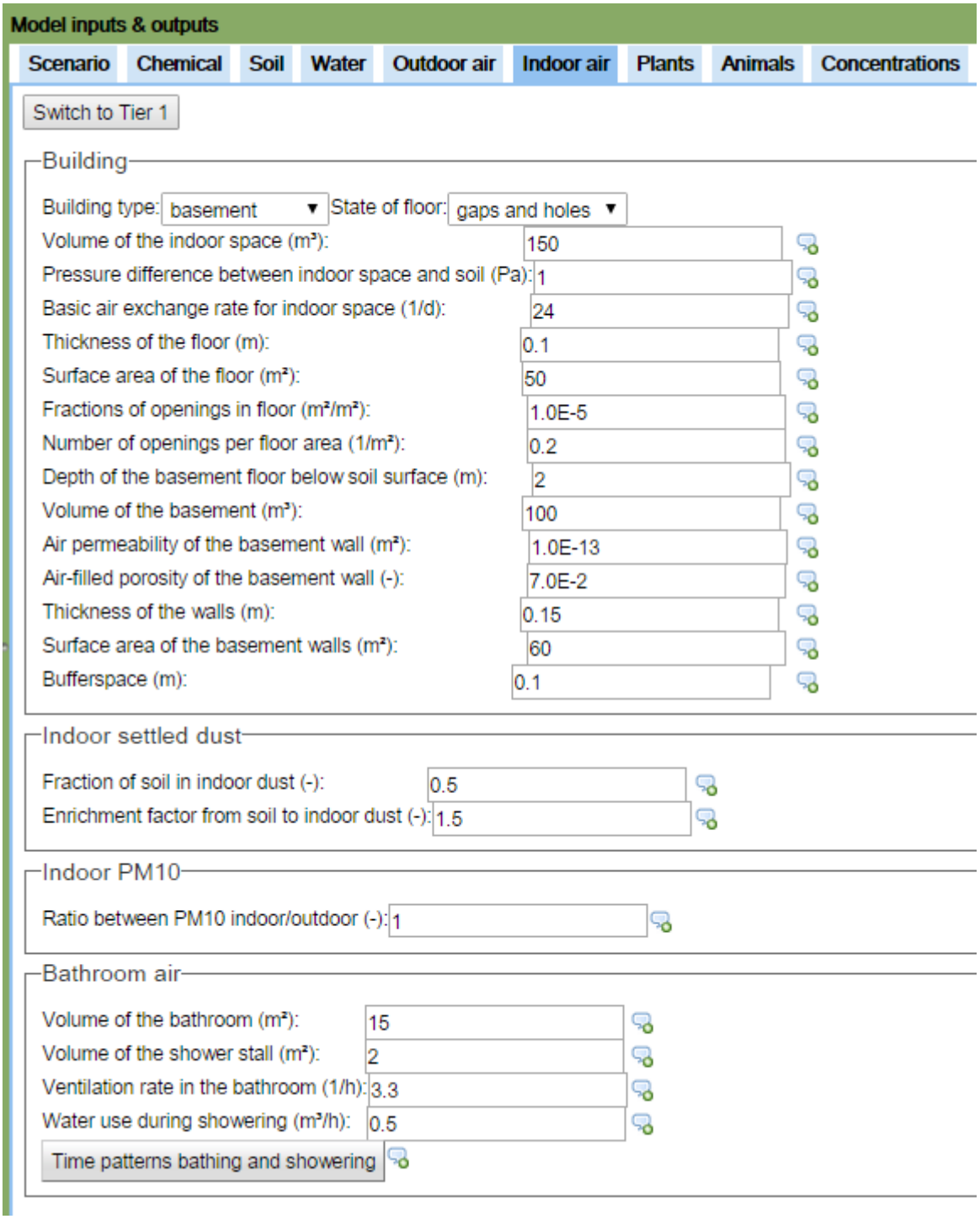


Figure 26: Indoor air tab at Tier 2

4.6.1. VAPOUR INTRUSION

The vapour intrusion module of S-Risk calculates the concentration to indoor air of a building resulting from vapour intrusion. Vapour intrusion from soil and/or groundwater is calculated. Both processes diffusion and convection are modeled. The concentration in indoor air is calculated for each soil layer and for the groundwater layer. This lower limit for this concentration is the ambient

air concentration. The highest concentration is taken forward in the exposure calculations (after addition of the concentration resulting from soil resuspension and particle intrusion). The vapour intrusion tab allows the selection of a building type from the "**Building type**" drop-down menu. You can choose between:

- *basement*: a basement with concrete floor, the calculations assume that basement and building form one space; there is no limitation on the exchange between basement and indoor air;
- *slab-on-grade*: building without basement, but with a concrete floor in contact with soil;
- *crawl space*: a building with a crawl space, the floor of the crawl space is formed by the soil layer below it; the crawl space is considered as a separate compartment with a calculated flux from crawl space to indoor air.

The option of a crawl space with concrete floor is not provided in the model yet. If you would like to perform calculations for a crawl space with concrete floor, you can perform a two-step approach, by first selecting the basement option, and then entering the dimensions of the crawl space (as if the total building had crawl space dimensions) and appropriate parameter values for ventilation of the crawl space. In a second run, a crawl space is selected and the indoor situation is parameterized as appropriate for the site. The resulting indoor air concentration from the first run can then – in the second run – be filled in as if it was a measured crawl space concentration in the Concentrations tab.

A second choice to be made is the "**State of floor**" menu. This choice is only needed for *basement* and *slab-on-grade* type buildings and relates to the concrete layer in contact with the soil. You can choose between "gaps and holes" or "intact floor". "Gaps and holes" is the default setting. Intact floor can be used for new floors in a perfect state. In that case, you preferably fill in the values for floor parameters to those corresponding to good or perfect floor quality.

Note: Under default settings and in a situation where diffusion dominates the vapour intrusion process (e.g., soils with low permeability, contamination at higher depth), it is possible that the option "intact floor" results in higher indoor air concentrations than the option "gaps and holes". This is a consequence of the modelling concepts behind the options. In case of "gaps and holes", diffusion takes place through larger holes covering only a small area of the total floor area. In case of "intact floor", diffusion takes place through small pores, but covering a relatively larger floor area. We therefore recommend to use "intact floor" only in combination with settings for good/very good floor quality. Of course, this should only be done when the site-specific situation allows for this choice.

→ **Tier 1**

Basement and slab-on-grade

Parameter	Building type	Information
volume of the indoor space	basement slab-on-grade	• Site-specific • Assumed to relate to ground-floor only.
depth of the basement /concrete slab floor below soil surface	basement slab-on-grade	• Site-specific

Parameter	Building type	Information
thickness of the floor	basement slab-on-grade	• Site-specific • Floor in contact with the soil.
surface area of the floor of the basement/slab	basement slab-on-grade	• Site-specific
volume of the basement	basement	• Site-specific
thickness of basement walls	basement	• Site-specific
surface area of basement walls	basement	• Site-specific

Crawl space

Parameter	Information
volume of the indoor space	• Site-specific • Assumed to relate to ground-floor only.
depth of the crawl space below soil surface	• Site-specific
thickness of the floor	• Site-specific • Relates to floor between crawl space and indoor.
surface area of the floor of the crawl space	• Site-specific
volume of the crawl space	• Site-specific
surface area of the crawl space walls	• Site-specific
thickness of crawls space walls	• Site-specific

→ **Tier 2**

In Tier 2, the parameter "*buffer space*" is visible. This parameter is used in the calculation of indoor air concentrations following vapour intrusion. It is the minimum distance between the top of the contaminated layer and the building when the flux from soil to the building (basement, crawl space, building) is calculated. The value is made visible to enable interpretation of application I results by running application II as the default value in application I (0.75 m) is different from that in application II or III (0.10 m). The value *should not be changed* for any other purpose.

Attention: The sum of the depth of the building (slab, basement or crawl space floor) and the length of the buffer space may at most be equal to the depth of the groundwater table. This condition results from the indoor air equations. These do not allow the calculation of vapour intrusion when the bottom of the basement is under groundwater level.

Basement and slab-on-grade, option gaps and holes

Parameter	Building type	Information
pressure difference between indoor space and soil	basement slab-on-grade	• Default value, recommended not to change this value except if well documented.
basic air exchange rate for indoor space	basement slab-on-grade	• Default, value is land use specific. • Background information is provided in the technical guidance document.
fractions of openings in floor	basement slab-on-grade	• Default: 'normal floor quality'. • Guidance as a function of floor quality is given in the technical guidance document. • Relates to the basement floor/concrete slab.
number of openings per floor area	basement slab-on-grade	• Default, recommended not to change. • Relates to the basement floor/concrete slab.
air permeability of basement wall	basement	• Default: 'good wall quality'. • Guidance as a function of wall material is given in the technical guidance document.
air-filled porosity of basement wall	basement	• Default: 'good wall quality'. • Guidance as a function of wall material is given in the technical guidance document.

Basement and slab-on-grade, option intact floor

Parameter	Building type	Information
pressure difference between indoor space and soil	basement slab-on-grade	• Default value, recommended not to change this value except if well documented.

Parameter	Building type	Information
basic air exchange rate for indoor space	basement slab-on-grade	• Default, value is land use specific. • Background information is provided in the technical guidance document.
air permeability of the intact floor	basement slab-on-grade	• Default: 'average floor quality'. • Guidance as a function of floor quality is given in the technical guidance document. • Relates to the basement floor/concrete slab.
air-filled porosity of the intact floor	basement slab-on-grade	• Default: 'average floor quality'. • Guidance as a function of wall material is given in the technical guidance document. • Relates to the basement floor/concrete slab.
air permeability of basement wall	basement	• Default: 'good wall quality' • Guidance as a function of wall material is given in the technical guidance document.
air-filled porosity of basement wall	basement	• Default: 'good wall quality' • Guidance as a function of wall material is given in the technical guidance document.

Crawl space

Parameter	Information
depth of the crawl space below soil surface	• Site-specific
pressure difference between crawl space and soil	• Default value, recommended not to change this value except if well documented.
pressure difference between indoor space and crawl space	• Default value, recommended not to change this value

Parameter	Information
	except if good arguments.
basic air exchange rate for crawl space	• Default, may be modified.
basic air exchange rate for indoor space	• Default, value is land use specific. • Background information is provided in the technical guidance document.
fractions of openings in floor	• Default: 'average floor quality'. • Guidance as a function of floor quality is given in the technical guidance document. • Relates to the floor between crawl space and indoor space.
number of openings per floor area	• Default, recommended not to change. • Relates to the floor between crawl space and indoor space.
air permeability of crawl space wall	• Default: 'good wall quality'. • Guidance as a function of wall material is given in the technical guidance document.
air-filled porosity of crawl space wall	• Default: 'good wall quality'. • Guidance as a function of wall material is given in the technical guidance document.
thickness of crawl space wall	• Site-specific

4.6.2. OTHER INDOOR PARAMETERS

The indoor air parameters related to the prediction of the concentration in indoor settled dust, the concentration on soil-derived indoor PM_{10}, and in bathroom air due to evaporation from water during showering are only editable under Tier 2.

Parameter	Information
fraction of soil in indoor dust	• Default, recommended not to modify unless good justification. • Land-use specific
enrichment factor from soil to indoor dust	• Default, recommended not to modify unless site-specific information is available.

Parameter	Information
	• Not independent from fraction of soil in indoor dust when site information is used.
ratio between indoor/outdoor PM10	• Default, recommended not to modify unless site-specific information.
volume of the bathroom	• Default
volume of the shower stall	• Default
ventilation rate in the bathroom	• Default • Based on ventilation recommendations.
water use during showering	• Default

The time patterns for bathing and showering can be modified by clicking the "**Time patterns bathing and showering**" button on the bottom of the screen. It is recommended not to change these values without good justification.

4.7. PLANTS TAB

The plants tab should only be looked at if there is either exposure of cattle or chicken or consumption of local vegetables by residents. The plants tab allows you to:

a) Specify chemical-specific transfer factors for vegetables and animal feed plants, and
b) Modify plant properties.

The chemical-specific factors are only accessible in case of a customized or newly added chemical. At Tier 1, the tab shows you three parameters values: volumetric washout factor for particles, metabolisation rate and photodegradation rate. A table, giving the overview of the way the concentration in the plant is calculated for each plant or plant type is visible as well (Figure 27).

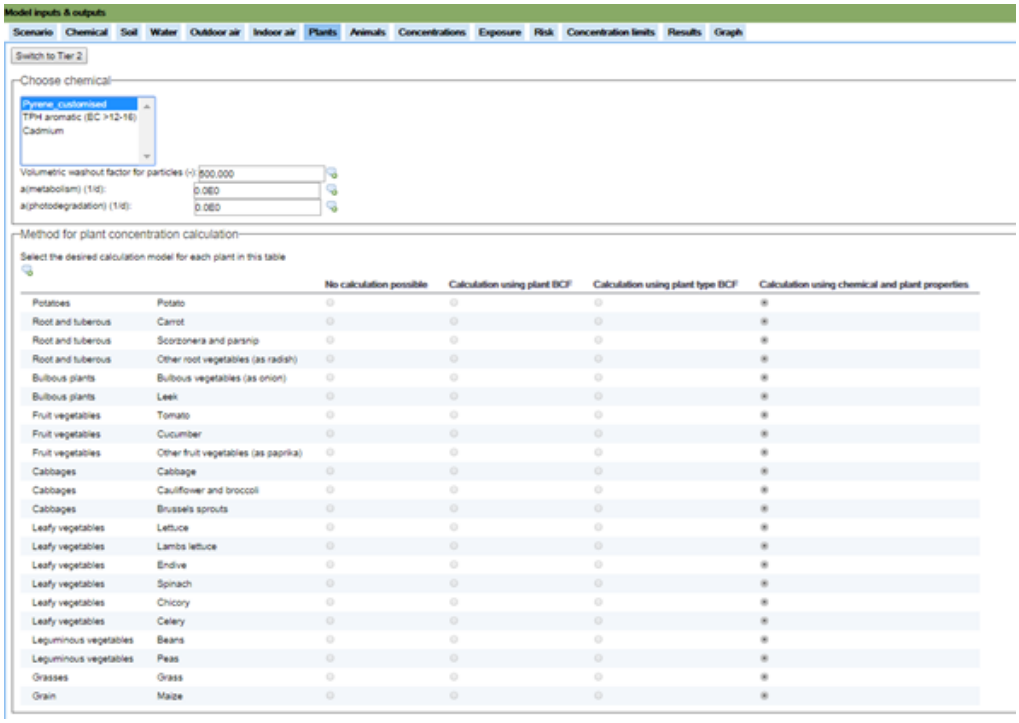


Figure 27: Plants tab at Tier 1 with customized chemical selected

The three parameters can be modified at Tier 1, under the condition of a new or customized chemical.

Parameter	Information
volumetric washout factor for particles	• Generic default value of 500 000. • In principle chemical-specific. • Factor used in the calculation of particle deposition on above-ground plant parts.
a(metabolism)	• Generic default value of 0. • Metabolization rate in the plant.
a(photodegradation)	• Generic default value of 0. • Photodegradation rate in above-ground plant parts.

The "**method for plant concentration calculation**" box gives a summary of how plant transfer is calculated for each of the vegetables (plants) and/or vegetable groups (plant types) on the screen. The table shows you the list of vegetables that is built in the model (2nd column). Each vegetable belongs to a vegetable group or plant type (1st column). With regard to animal exposure, grass and maize are provided. Then, four columns are available that indicate which option for plant transfer calculation is selected:

- *No calculation possible*: no selection available on BCF model to be used, calculation of plant transfer will not be possible;

- *Calculation using plant BCF*: a plant transfer factor (bioconcentration factor or BCF) is filled in at the level of the plant;
- *Calculation using plant type BCF*: a plant transfer factor (bioconcentration factor or BCF) is filled in at the level of plant type; the BCF will then automatically be assigned to the vegetables belonging to that plant type;
- *Calculation using chemical and plant properties*: this option is only available for organic chemicals; no BCF has to be filled in and plant transfer will be calculated by the model, using chemical-specific properties (K_{ow}, K_{oa}, H) and plant properties (see plant characteristics).

The information behind this summary table can – for a customized or newly added chemical - be accessed under Tier 2 by clicking the "**Add or adjust available BCF models**" button. For a default chemical, the information can only be viewed. At Tier 2, also the button "**Plant characteristics**" becomes visible (Figure 28).

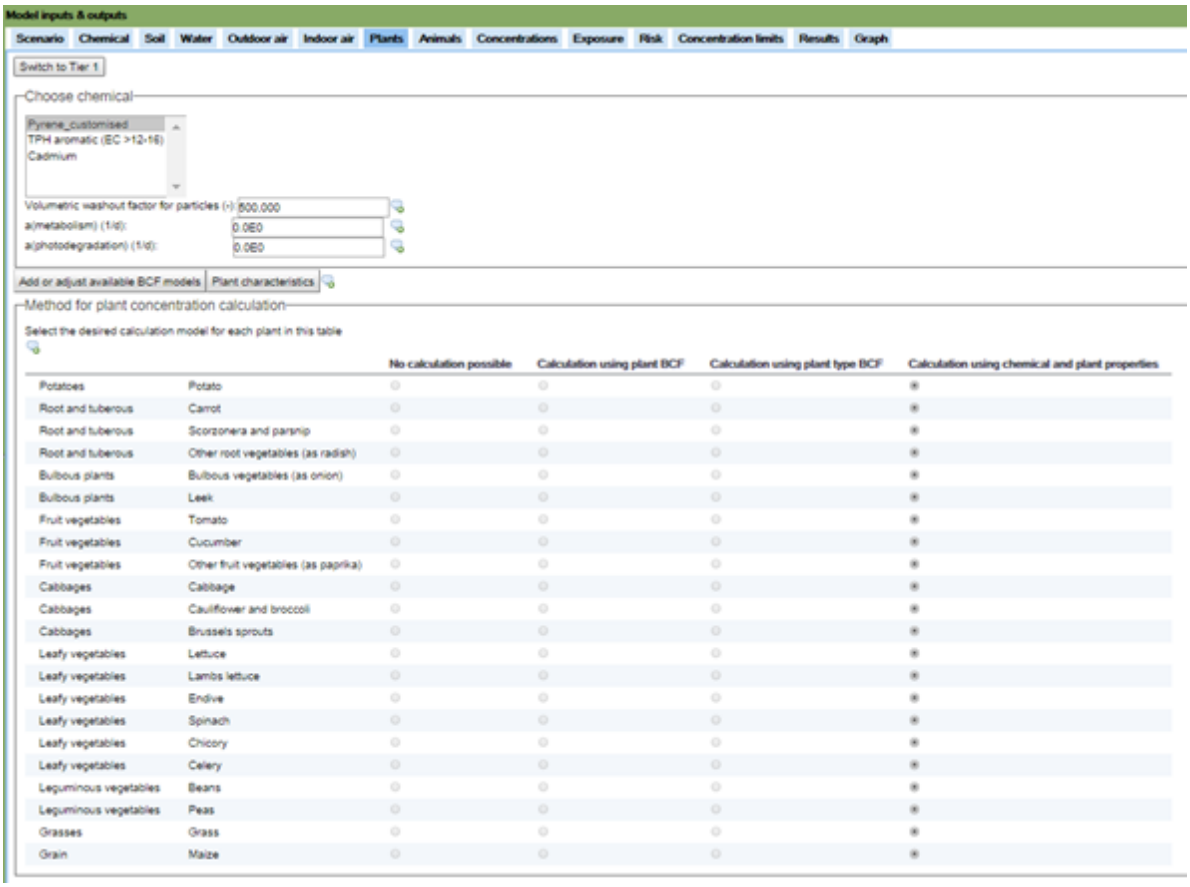


Figure 28: Plants tab at Tier 2 with customized chemical selected, indicating the BCF models and Plant characteristics buttons

4.7.1. MODIFYING PLANT TRANSFER PROPERTIES (TIER 2)

→ Organic chemicals

To modify the plant transfer properties for organic chemicals, you first select the chemical for which you want to modify the data and then indicate for each plant/plant type whether you want

to fill in / modify the data at plant type or plant level ("**planttype /plant**" box) in the menu. You can then specify the data in the "Available model for plant / plant type" menu (Figure 29).

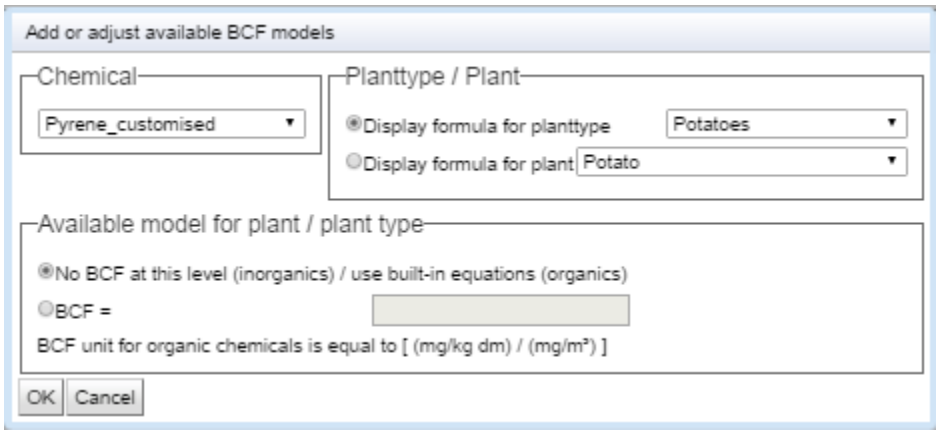


Figure 29: Menu for available BCF models for organic chemicals

There are two options for organic chemicals:

- Use built-in equations: if you select this option, the concentration in the plant for that plant or plant type will be calculated by the model using chemical and plant properties;
- BCF: if you have a BCF value for the plant or plant type, you can fill the value in; note that the units are mg/kg dm in the plant per mg/m³ soil solution.

It is necessary that a selection is made for each plant or at least plant type.

→ **Inorganic chemicals**

To modify the plant transfer properties for inorganic chemicals, you first select the chemical for which you want to modify the data and then indicate for each plant/plant type whether you want to fill in / modify the data at plant type or plant level ("**planttype /plant**" box) in the menu. You can then specify the data in the "Available model for plant / plant type" menu (Figure 30).

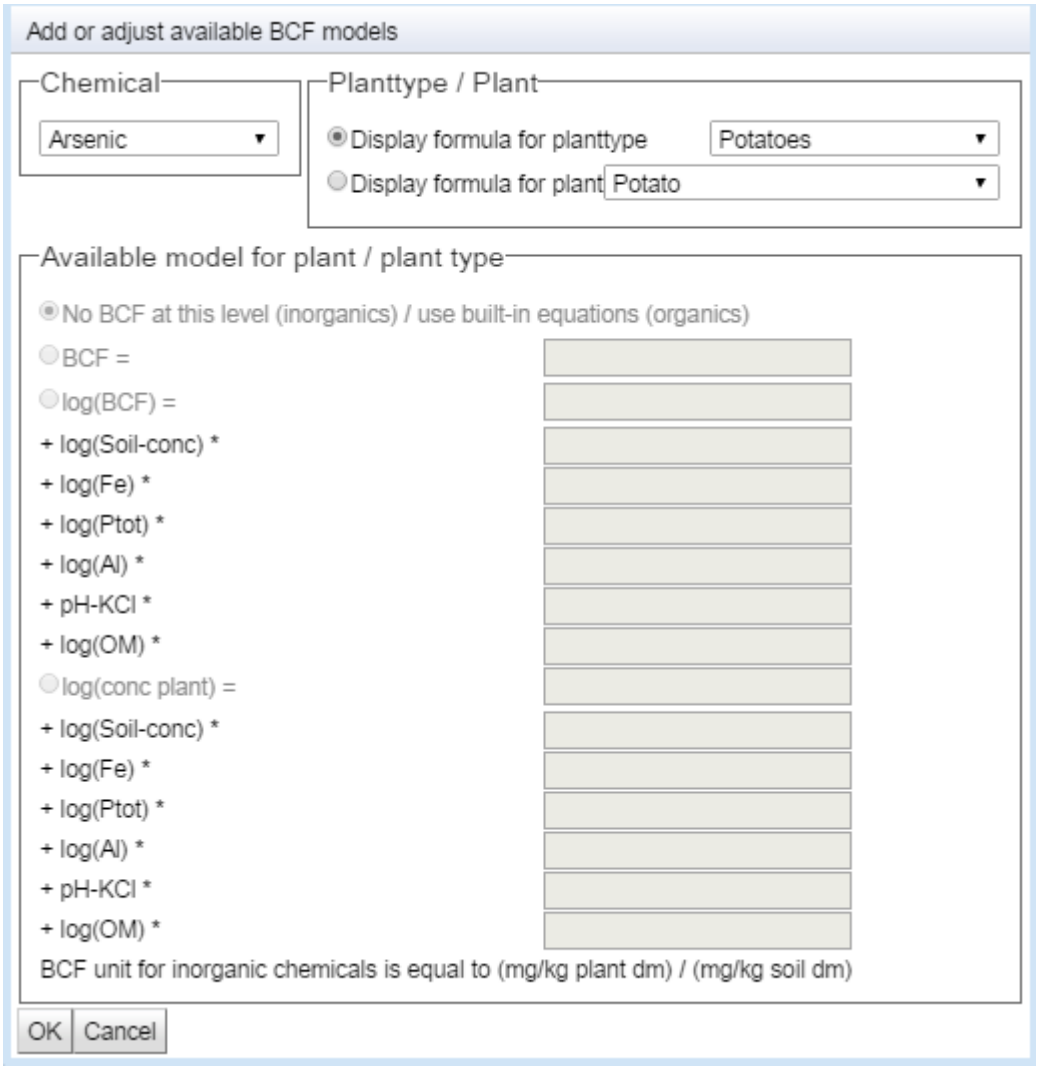


Figure 30: Menu for BCF models for inorganic chemicals

For inorganic chemicals it is required to fill in a BCF either at plant level or at plant type level. The model has no equations to estimate the BCF value. As an example from Figure 30, the plant type potatoes has no BCF, as indicated by the marked radio button "**No BCF at this level**". In that case, there will be a BCF value at the level of the plant potatoes. Vice versa, it is possible to have the radio button "**No BCF at this level**" marked for a plant, but then there needs to be a BCF at plant type level. There are three options to fill in a BCF at either plant or plant type level:

- BCF: a single BCF value can be filled in;
- Log (BCF): a BCF relation can be filled in, this relation expresses the log BCF as a function of the log of the soil concentration and a number of soil-related parameters; an intercept and slope factors are required (they can be 0);
- Log (conc plant): a plant relation can be filled in, this relation expresses the log of the plant concentration as a function of the log of the soil concentration and a number of soil-related parameters; an intercept and slope factors are required (they can be 0).

The unit of the BCFs for inorganic chemicals is mg/kg dm in the plant per mg/kg dm in the soil.

4.7.2. MODIFYING PLANT PROPERTIES (TIER 2)

Plant properties can be modified by clicking the "**plant characteristics**" button on the plants tab at Tier 2. You will get access to a menu with the list of plants and their properties (Figure 31).

Plant characteristics

	Q	k	L	f_ch	t	ρ	A	y_v	dm	r_p
Potato		1,39E-1	1,5E-3	1,9E-1	1,28E2	1,02E3		3,897E0	2,0E1	4,0E-2
Carrot	7,78E-4	1,0E-1	2,5E-2		1,2E2	1,02E3		5,2E0	1,1E1	
Scorzonera and parsnip	2,71E-4	1,0E-1	2,5E-2		1,2E2	1,02E3		2,5E0	9,0E0	
Other root vegetables (as radish)	1,292E-3	1,0E-1	2,5E-2		2,9E1	8,2E2		2,0E0	5,0E0	
Bulbous vegetables (as onion)	1,008E-3	3,5E-2	2,5E-2		5,5E1	8,0E2	5,0E0	3,4E0	1,1E1	
Leek	1,563E-3	3,5E-2	2,5E-2		1,79E2	8,0E2	5,0E0	3,0E0	1,3E1	
Tomato	6,58E-4	3,5E-2	2,5E-2		1,5E2	8,0E2	5,0E0	3,97E1	5,0E0	
Cucumber	6,58E-4	3,5E-2	2,5E-2		1,5E2	8,0E2	5,0E0	3,38E1	4,0E0	
Other fruit vegetables (as paprika)	6,58E-4	3,5E-2	2,5E-2		1,5E2	8,0E2	5,0E0	1,62E1	9,0E0	
Cabbage	6,58E-4	3,5E-2	2,5E-2		9,1E1	8,0E2	5,0E0	5,5E0	8,0E0	
Cauliflower and broccoli	1,0E-3	3,5E-2	2,5E-2		9,1E1	8,0E2	5,0E0	2,4E0	8,1E0	
Brussels sprouts	5,12E-4	3,5E-2	2,5E-2		1,17E2	8,0E2	5,0E0	1,8E0	1,7E1	
Lettuce	1,225E-3	3,5E-2	2,5E-2		6,9E1	6,1E2	5,0E0	4,4E0	4,0E0	
Lambs lettuce	4,42E-4	3,5E-2	2,5E-2		6,9E1	6,5E2	5,0E0	1,0E0	4,0E0	
Endive	9,25E-4	3,5E-2	2,5E-2		6,9E1	7,35E2	5,0E0	5,0E0	6,2E0	
Spinach	1,225E-3	3,5E-2	2,5E-2		6,9E1	6,3E2	5,0E0	2,0E0	8,0E0	
Chicory	5,63E-4	3,5E-2	2,5E-2		7,3E1	7,0E2	5,0E0	1,5E0	6,0E0	
Celery	3,92E-4	3,5E-2	2,5E-2		1,2E2	8,0E2	5,0E0	6,3E0	8,0E0	
Beans	3,92E-4	3,5E-2	2,5E-2		7,7E1	8,0E2	5,0E0	2,5E0	1,1E1	
Peas	5,33E-4	3,5E-2	2,5E-2		9,5E1	8,0E2	5,0E0	8,0E-1	1,8E1	
Grass	1,563E-3	3,5E-2	2,5E-2		3,0E1	8,2E2	5,0E0	5,93E0	3,5E1	
Maize	1,2E-3	3,5E-2	5,4E-2		1,83E2	8,0E2	5,0E0	4,53E0	2,5E1	

OK Cancel

Figure 31: Plant characteristics table (Tier 2)

Parameter	Information
Q – transpiration rate	• in case of organic chemicals and transfer calculated using chemical and plant properties.
k – growth rate	• in case of organic chemicals and transfer calculated using chemical and plant properties. • default value from model concept.
L – lipid content	• in case of organic chemicals and transfer calculated using chemical and plant properties.
f_ch – carbohydrate content	• in case of organic chemicals and transfer calculated using chemical and plant properties. • only used for potatoes.
t – plant growth period	• soil to plant transfer for organic chemicals and transfer calculated using chemical and plant properties. • deposition calculations for all chemical types.
ρ – plant density	• in case of organic chemicals and transfer calculated using chemical and plant properties.

Parameter	Information
A – surface area of aboveground plant parts	• in case of organic chemicals and transfer calculated using chemical and plant properties.
Y_v - plant yield	• in case of organic chemicals and transfer calculated using chemical and plant properties. • deposition calculations for all chemical types.
dm – dry matter content	• used to convert calculated concentrations at dry matter to concentration at fresh weight for exposure calculations.
r_p – radius of a potato	• in case of organic chemicals and transfer calculated using chemical and plant properties.

4.8. ANIMALS TAB

The animals tab is only of importance if there is exposure of animals (cattle, sheep, chicken) on a farm or for local consumption. The animals tab allows you to:

a) Modify cattle and chicken exposure parameters (time pattern, feed pattern);
b) Enter or modify transfer factors to animal products for new or customized chemicals.

At Tier 1, you will be able to change the contribution of water sources that are used as drinking water for cattle, sheep and chicken. The latter only in case you included chicken eggs as an exposure pathway in a customized scenario. In addition, when dealing with a newly defined or customized chemical, you will have access to the fields for specification of the biotransfer factors (BTF).

Concentrations in cattle and in chicken eggs are taken forward to exposure calculations. Concentrations in sheep meat are only used to compare with concentration limits. Concentrations in chicken meat are not calculated by the model.

4.8.1. MODIFICATION OF CATTLE AND CHICKEN EXPOSURE PARAMETERS

→ **Tier 1**

At Tier 1 (Figure 32), it possible to modify:

- Drinking-water sources for chicken (if the local chicken egg consumption exposure pathway is active);
- Drinking-water sources for cattle and sheep.

You can specify the fraction of groundwater and the fraction of supply-water. Depending upon your settings, the groundwater concentration is either calculated or entered, the supply-water concentration is calculated or can be overwritten in the Concentrations tab. If the sum of the fraction of groundwater and supply-water does not equal 1, the remaining fraction is assigned to "other water", for which a concentration has to be entered in the Concentrations tab. The final

water concentration is then a weighted average of the groundwater, supply-water and other water concentrations.

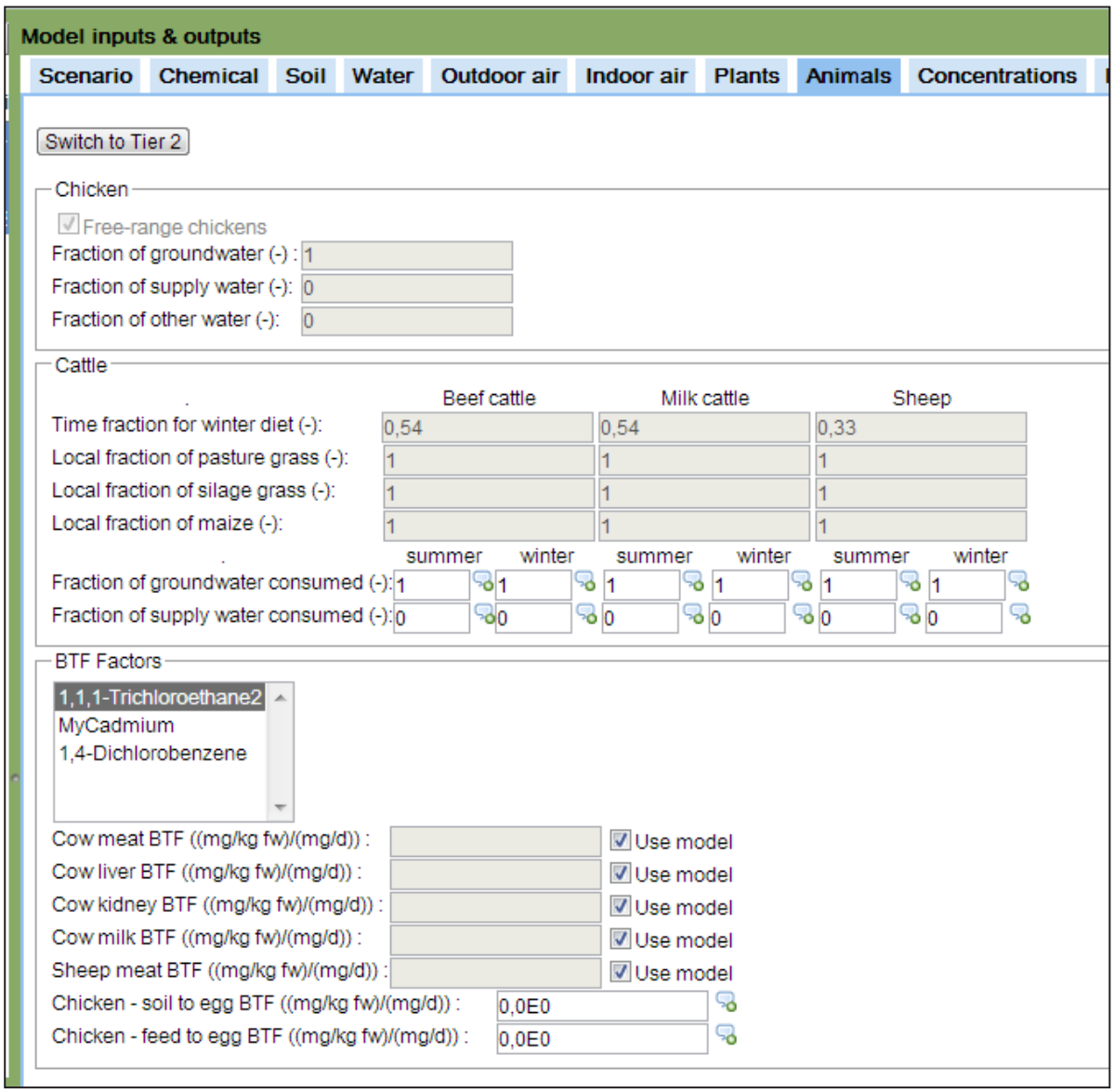


Figure 32: Animals tab at Tier 1

→ **Tier 2**

At Tier 2, all feed fields will become editable and an additional button "**Animal intake data**" will appear on the Animals tab (Figure 33).

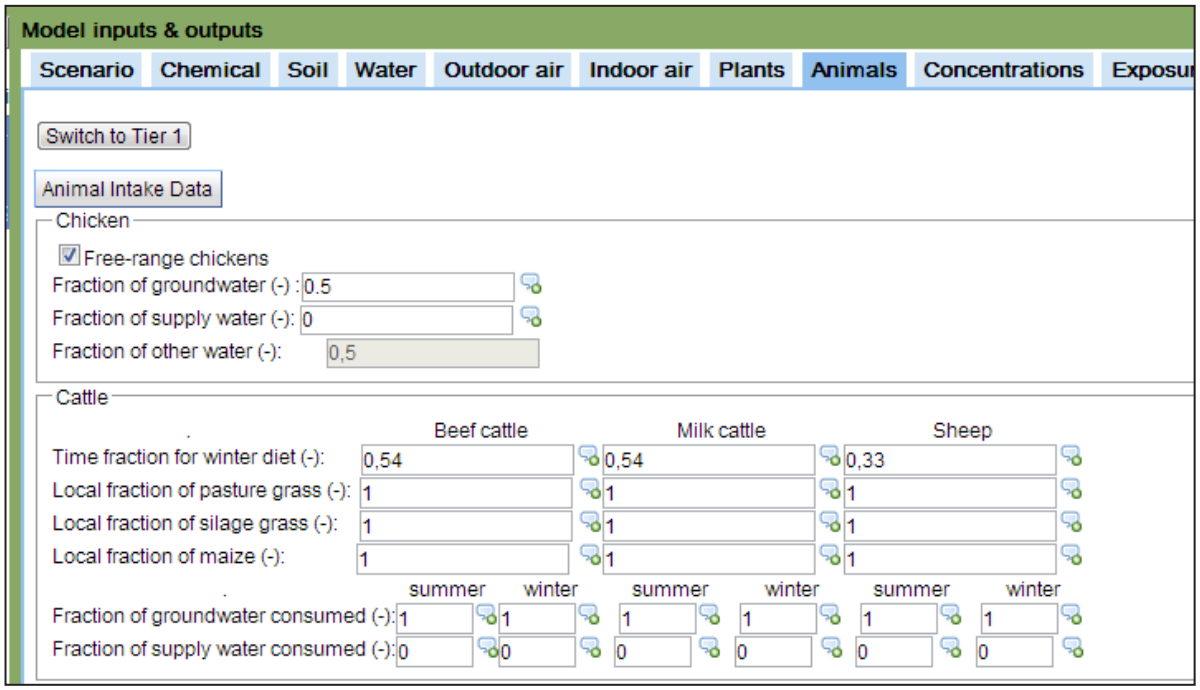


Figure 33: Animal parameters on Animals tab at Tier 2

Parameter	Information
time fraction of winter diet	• Time fraction (between 0 and 1) that the animal is fed the winter diet; time fraction for winter diet relates to the time in the stable during winter period.
local fraction of pasture grass	• Fraction (between 0 and 1) of pasture grass in diet that is coming from the site; the concentration for the local fraction is taken from the calculated or entered concentration in grass. • If the entered value for the local fraction is < 1, the concentration for the non-local fraction is taken from the Concentrations tab (background concentrations). • The animal exposure concentration is a weighted average of local and non-local concentration.
local fraction of silage grass	• Fraction (between 0 and 1) of silage grass in diet that is coming from the site; the concentration for the local fraction is taken from the calculated or entered concentration in grass. • If the entered value for the local fraction is < 1, the concentration for the non-local fraction is taken from the Concentrations tab (background concentrations). • The animal exposure concentration is a weighted average of local and non-local concentration.
local fraction of maize	• Fraction (between 0 and 1) of maize in diet that is coming from the site; the concentration for the local fraction is

Parameter	Information
	taken from the calculated or entered concentration in maize. • If the entered value for the local fraction is < 1, the concentration for the non-local fraction is taken from the Concentrations tab (background concentrations). • The animal exposure concentration is a weighted average of local and non-local concentration.

When you click the "**Animal intake data**" button, a table will open (Figure 34). This table will allow you to enter site-specific information with regard to summer and winter diet of cattle and sheep, and of the diet of chicken.

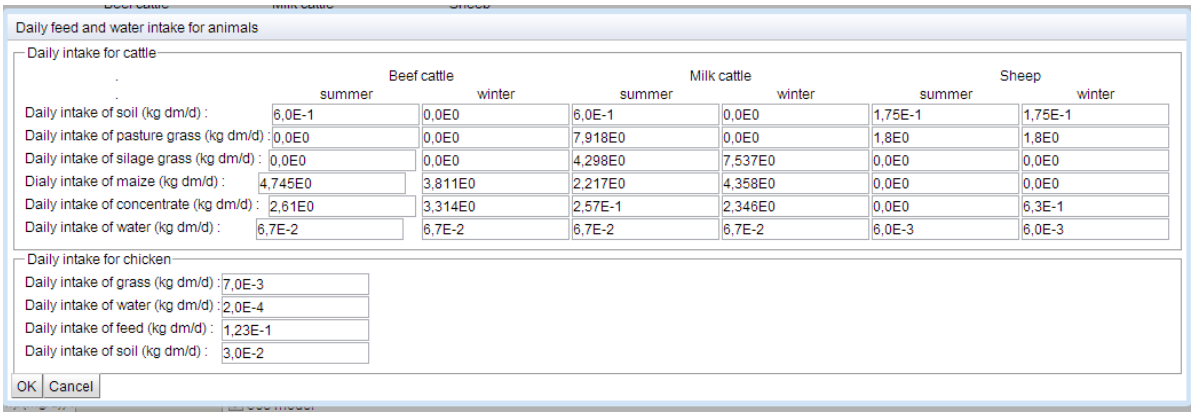


Figure 34: Feed intake table on Animals tab at Tier 2

Parameter	Information
daily intake of soil - cattle	• Recommended not to change the value except if well-documented. • Uses the concentration in topsoil from the soil profile or the separately entered soil-animal concentration (see Concentrations tab).
daily intake of pasture grass - cattle	• Uses a weighted average of local grass concentration (calculated or entered) and non-local pasture grass concentration.
daily intake of silage grass - cattle	• Uses a weighted average of local grass concentration (calculated or entered) and non-local silage grass concentration.
daily intake of maize - cattle	• Uses a weighted average of local maize concentration (calculated or entered) and non-local maize concentration.
daily intake of concentrate - cattle	• Is not related to the local site, but uses an entered

Parameter	Information
	background concentration (Concentrations tab).
daily intake of water - cattle	• Uses a weighted concentration of groundwater (calculated or entered), supply water (calculated or entered) and other water (entered) concentration.
daily intake of grass – chicken	• Uses a weighted average of local pasture grass concentration (calculated or entered) and non-local pasture grass concentration.
daily intake of water – chicken	• Uses a weighted concentration of groundwater (calculated or entered), supply water (calculated or entered) and other water (entered) concentration.
daily intake of feed – chicken	• Is not related to the local site, but uses an entered background concentration (Concentrations tab).
daily intake of soil – chicken	• Default value represents a worst-case; guidance for value choice as a function of available area and soil coverage is given in the technical guidance document. • Uses the concentration in topsoil from the soil profile or the separately entered soil-animal concentration (see Concentrations tab).

4.8.2. MODIFICATION OF BIOTRANSFER FACTORS

Concentrations in animal products are calculated with biotransfer factors (BTF). These express the ratio between the concentration in the animal product and the total intake. For inorganic chemicals, the BTF values are always required parameters. For organic chemicals, the BTF values can be filled in, but can also be calculated using a BTF model for meat and dairy products. The calculation is done using the log Kow of the chemical. For chicken eggs, a model is not implemented yet and thus BTF values should be filled in for all chemicals.

Attention: For default chemicals, the BTF values for chicken eggs are often set at 0 (except for some metals). This does not mean that no transfer to chicken eggs occurs, but that values are not looked up. So, if consumption of chicken eggs is activated as an exposure pathway, it is required that appropriate values are filled in, even for default chemicals.

4.9. CONCENTRATIONS TAB

The Concentrations tab allows you to:

a) Enter the soil concentrations according to the specified soil profile;
b) Enter the groundwater concentration if this option is chosen;
c) Enter pathway-specific soil concentrations;
d) Enter concentrations in transfer media;
e) Enter animal-related (background) concentrations.

The concentrations tab is shown in Figure 35. If Tier 1 is chosen, the "**Plants**" and "**Animals**" button will not be visible. To enter concentrations for a chemical in the list, click on the chemical and enter the corresponding concentrations as explained below.

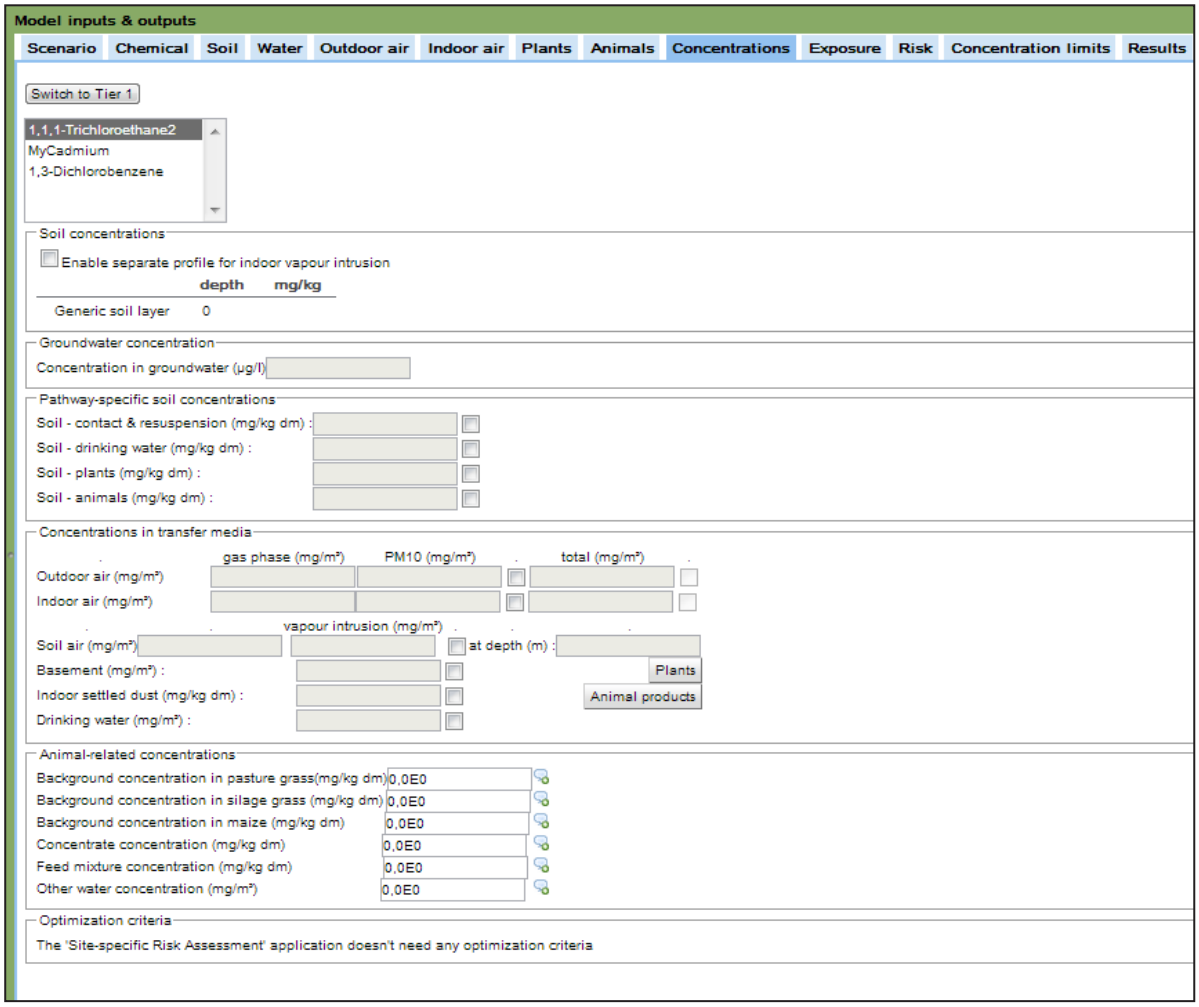


Figure 35: Concentrations tab at Tier 2

4.9.1. ENTERING SOIL AND GROUNDWATER CONCENTRATIONS

→ Soil profile

The soil concentrations corresponding to the layers defined in the Soil tab, can be entered in the "**Soil concentrations**" panel. A table will be visible indicating the layers entered and their corresponding depth. Clicking the fields under the mg/kg heading, will allow you to enter the concentrations. The "Soil concentrations" panel has a checkbox, providing the possibility to "**Enable separate profile for indoor vapour intrusion**". This option can be used to enter different concentrations for the ambient transfer calculations and the vapour intrusion pathways. The soil type profile is equal for outdoor and indoor, but you will be able to enter a separate concentration profile for indoor vapour intrusion calculations (Figure 36).

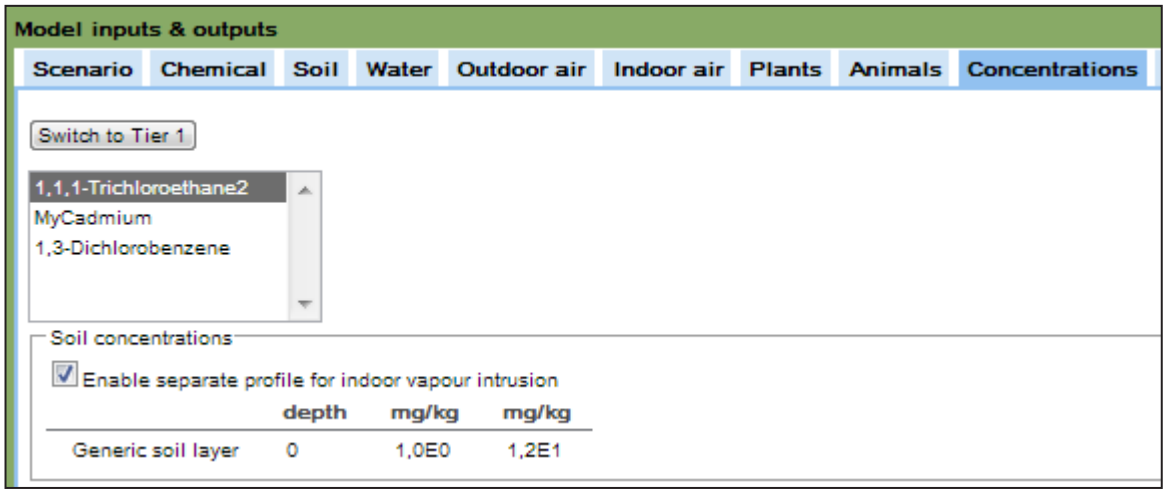


Figure 36: Entering separate concentration profiles for outdoor transfer calculations and vapour intrusion calculations

→ **Groundwater concentration**

If you have chosen the option to fill in a groundwater concentration (Migration to groundwater), the field to enter a concentration in the "**Groundwater concentration**" panel will be editable. If you have chosen to have the groundwater concentration calculated by the model, the field will be disabled.

4.9.2. ENTERING PATHWAY-SPECIFIC SOIL CONCENTRATIONS

If you would have soil concentrations that are different from the overall soil profile data and that are linked to specific exposure pathways, these concentrations can be entered in the panel "**Pathway-specific soil concentrations**". To do so, activate the checkbox at the right of the corresponding soil concentration to enable the concentration field. You can then enter the soil concentration (Figure 37).

Figure 37: Entering pathway-specific soil concentrations

The pathway-specific soil concentrations are used as follows:

- Soil – contact and resuspension: concentration to be used for soil ingestion, dermal contact with soil and soil resuspension (including subsequent transfer to the indoor environment);
- Soil – drinking water: concentration to be used to calculate the permeation through supply-water pipes; the properties of the layer corresponding to the depth of the supply-water pipe (as entered on the Water tab) will be used;

- Soil – plants: concentration to be used for plant uptake calculations (vegetables, grass and maize), replaces the default selection of the concentration of the top 30 cm of soil (which is a weighted average concentration of layers in case of differentiation in soil profile within 30 cm of depth);
- Soil – animals: concentration to be used for soil ingestion by animals.

4.9.3. ENTERING CONCENTRATIONS IN TRANSFER MEDIA

Concentrations in transfer media can be entered at Tier 1 for air (outdoor, indoor, soil and crawl space/basement), settled dust and drinking water. At Tier 2, concentrations in plants and animal products can be entered as well (Figure 38). You can enter the concentrations after activating the checkbox at the right of the corresponding field.

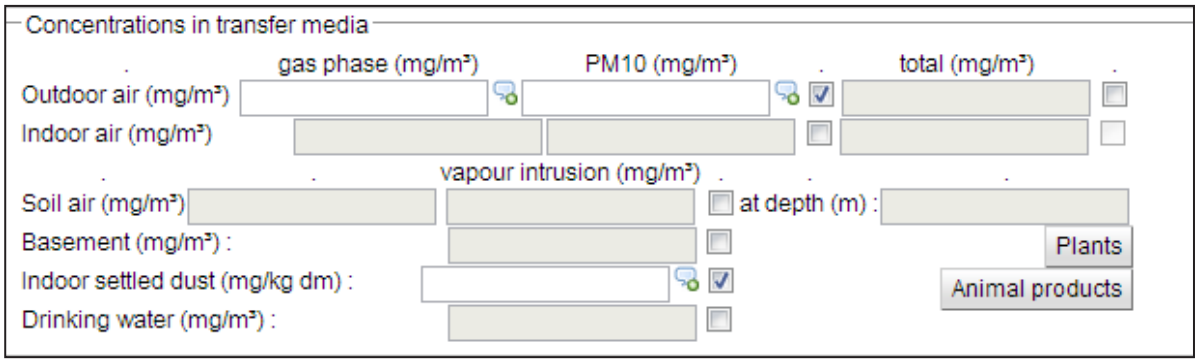


Figure 38: Entering concentrations in transfer media

→ **Outdoor air and indoor air**

Outdoor and indoor air concentrations can be entered in two ways: either as separately measured **concentrations in gas phase** and on **PM_{10}**, or as a total concentration in air. You have to fill in a value for both type of concentrations if you select the option for gas phase and PM_{10}. If you would have measured only the gas phase concentration or only the concentration on PM_{10}, and the chemical properties are such that the concentration on the other phase would be zero (or negligible), you can enter the measured concentration for the corresponding phase and fill in a zero value for the other phase.

If you enter the concentration as a **total concentration**, you first have the activate the checkbox at the right of the gas phase and PM_{10} fields and subsequently the checkbox at the right of the total field. This will make the total field accessible. If you enter a total concentration, the model will automatically distribute the concentration over gas phase and PM_{10} according to the equation given below. This is done as the model needs separate gas phase and PM_{10} concentrations for part of the transfer and exposure calculations.

$$C_{gas\ phase} = (1 - \varphi) \times C_{total,air}$$

$$C_{PM10} = \varphi \times C_{total,air}$$

where:

$C_{total,air}$ the total concentration in air [mg/m³]
$C_{gas\ phase}$ the gas phase concentration in air [mg/m³]

C_{PM10} the particle concentration in air [mg/m³]
ϕ the fraction adsorbed on atmospheric aerosol particles [-]

The fraction adsorbed on atmospheric aerosol particles is given by the Junge-Pankov model:

$$\varphi = \frac{c \times \theta}{p_{OL}(T) + c \times \theta}$$

where:

c the Junge-Pankov constant [Pa.m] = 0.17
θ the specific surface area of aerosol particles [m^2/m^3] = 1.1 x 10^{-3} (urban areas)
$p_{OL}(T)$ the subcooled liquid vapour pressure at ambient temperature T [Pa]

For compounds that are liquids at ambient temperature, the subcooled liquid vapour pressure is equal to the normal liquid vapour pressure at ambient temperature. We therefore use the chemical-specific vapour pressure (Chemicals tab) instead of the subcooled liquid vapour pressure to calculate the distribution over gas phase and particle phase.

The filled in concentrations will be used to overwrite model predictions.

→ **Soil air**

You can overwrite the predicted concentrations in soil air by filling in a value in the "**soil air**" field. If you have activated the option of a separate concentration profile for indoor vapour intrusion in the soil concentrations panel, you will be able here to fill in a separate soil air concentration for vapour intrusion as well. You need to fill in the depth at which the soil air concentration was measured as well.

When you enter a measured soil air concentration, this value will be the only value that is used in the volatilization calculations. It will replace all of the layer-dependent predicted concentrations.

→ **Crawl space/basement air**

If you have a measured concentration in crawl space or basement air, you can fill in this value on the concentrations tab.

Attention: As the model considers the basement and the ground floor of the building as one compartment, basement measurements cannot be added directly. If you still would have a basement measurement, you should change the building type into crawl space with appropriate settings for the quality of the floor (between crawl space and indoor). The quality of the floor should be set at bad quality (taking into account that in reality there is often little dilution between basement and indoor air). Information on the settings can be found in the technical guidance document. You can then enter the basement concentration as a crawl space concentration. Or you can enter the basement concentration as an indoor air concentration as a worst-case assumption.

In case of a slab-on-grade building, you will notice that there is a field for basement/crawl space concentrations, but this field is not accessible.

→ **Indoor settled dust**

A measured concentration in indoor settled dust can be entered. The relationship between the soil concentration and indoor settled dust, which is used by the model then gets lost. This is no problem if you make use of only one set of concentrations. If you know that – for your assessment – there is a relation between the concentration in soil and in indoor settled dust, you can also specify this relationship in the Indoor air tab by entering appropriate values for the fraction of soil in indoor settled dust and the enrichment factor from soil to indoor settled dust.

→ **Drinking water**

The entered concentration in drinking water will override the calculated concentration in drinking water as a result of permeation through supply-water pipes.

→ **Plants and animal products**

You can override predicted concentrations in plants and in animal products by clicking the "**Plants**" and the "**Animal products**" button, respectively. When the table for plants opens, you need to click the chemical for which you enter data, after which a table with vegetables, grass and maize will appear (Figure 39). You can then enter values in the corresponding fields for the selected chemical.

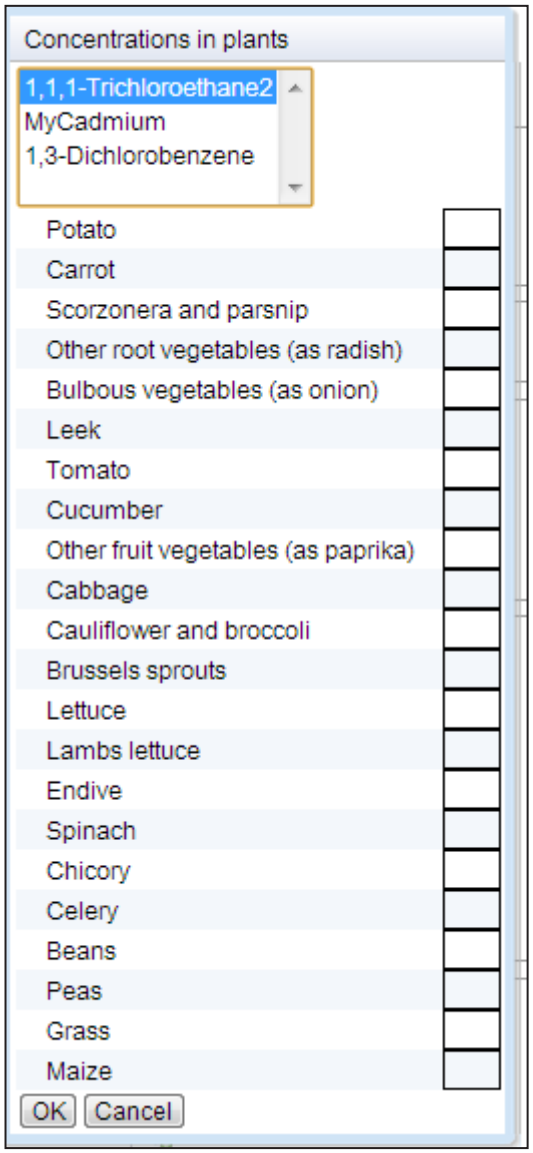


Figure 39: Entering concentrations in plants (Tier 2)

When you click the button for Animal products, a panel will be shown (Figure 40). After selecting the chemical for which you want to enter concentration, the fields corresponding to the animal products will become editable.

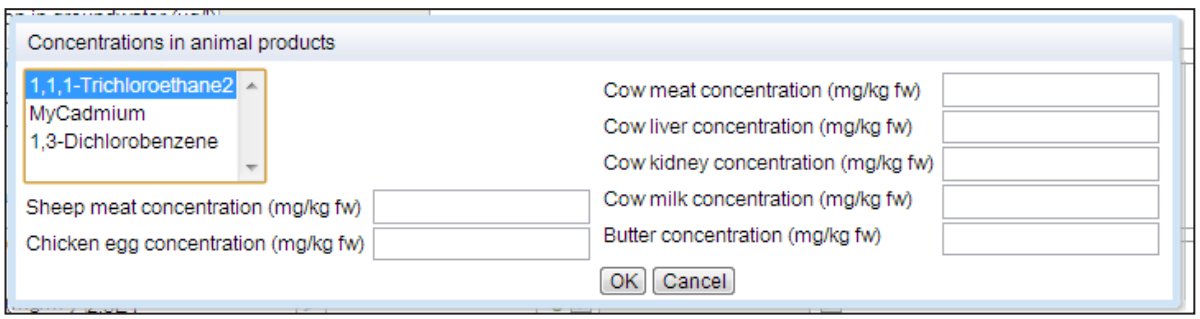


Figure 40: Entering concentrations in animal products (Tier 2)

4.9.4. ENTERING ANIMAL-RELATED CONCENTRATIONS

The panel called "**Animal-related concentrations**" will have accessible fields when you have a newly defined or customized chemical. The animal-related concentrations are only relevant if you want to calculate exposure through animal products and/or chicken eggs. By default, they are set at 0, meaning that only local exposure of cattle is accounted for.

The concentrations relate to background concentrations that are used for the fraction of the feed that is not from local origin. The concentrate concentration (cattle) and feed concentration (chicken) is always used (as concentrate and feed is never considered to be of local origin). The concentration in other water is used if you have specified that not all water for cattle/chicken is groundwater or supply-water (i.e., the sum of the fractions of groundwater and supply-water is smaller than 1).

4.10. EXPOSURE TAB

Exposures calculated are daily (except food) and yearly averages. For dietary exposure, only yearly averages are calculated (as the consumption figures are yearly averages). Fields in the exposure tab are only accessible in case of a newly defined or customized chemical. In case of a default chemical, the values are visible but cannot be modified. When you view the exposure tab at Tier 2, you will have an additional button called "Adjust age-specific weight factors". Consumption figures and fractions of locally produced foods will become visible and editable as well (also for default chemicals) (Figure 41).

S-Risk takes into account background exposure in the risk characterization for *threshold effects*, for which the risk is calculated using a TDI approach (see Risk tab). Background exposures via food and drinking-water are added to local oral exposure; background exposure via inhalation is added to local inhalation exposure. If you would use measured concentrations for drinking-water, ambient or indoor air, you need to be aware of the fact that the overall background is added for these threshold effects. In order to avoid double-counting, you should either correct the measured concentration or you set the background concentration equal to 0. This correction is not required for measured concentrations in food and feed as here double-counting is not possible.

In case of chemicals with only non-threshold or pseudo-threshold effects considered, the background exposure is of less importance, as it is not accounted for in the risk characterization.

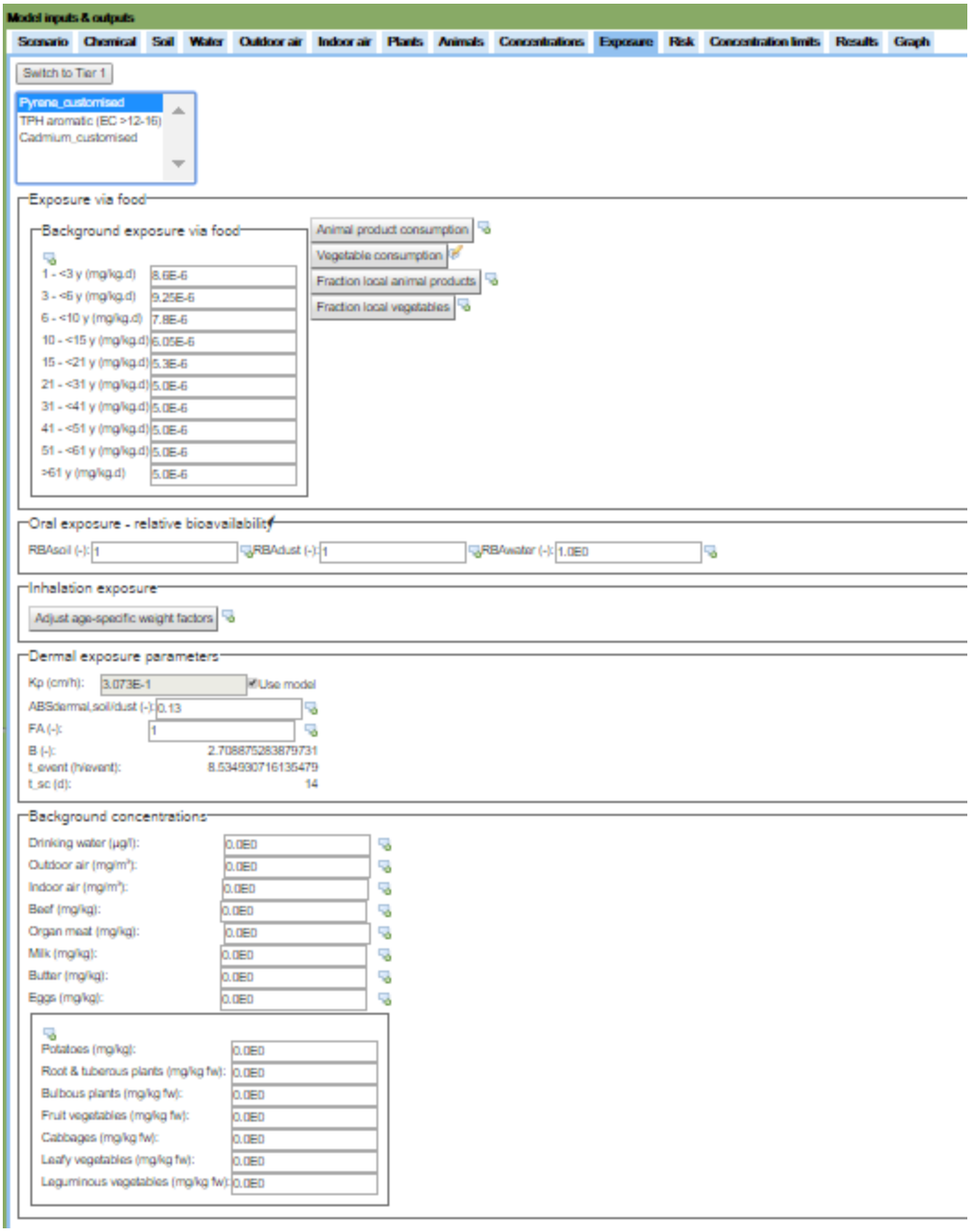


Figure 41: Exposure tab at Tier 2

4.10.1. BACKGROUND EXPOSURE VIA FOOD

Background exposure via food requires age-dependent values. If you have such values available, you can enter them here. In many cases, however, there is only information available for adults (or for a limited number of age categories). In that case, the age-dependent background exposure from diet (excluding drinking-water) for adults can be used to estimate background exposure at other ages by multiplying the adult intake (mg/kg.d) with following relative ratios:

age	1 - < 3yr	3 - < 6 yr	6 - < 10 yr	10 - < 15 yr	15 - < 21 yr	21 – 31 yr	31+ yr
ratio	1.72	1.85	1.56	1.21	1.06	0.99	1.00

4.10.2. CONSUMPTION FIGURES AND FRACTIONS OF LOCALLY PRODUCED FOODS

At Tier 2, four buttons become visible within the "Exposure via food" panel: animal product consumption, vegetable consumption, fraction local animal products and fraction local vegetables. These buttons comprise the consumption figures and fractions of locally produced foods that are considered when the exposure pathways "intake via locally produced vegetables", "intake via locally produced meat and milk" and/or "intake via locally produced eggs" are checked on the "Scenario" tab.

4.10.3. ORAL EXPOSURE – RELATIVE BIOAVAILABILITY

The calculations allow to take into account differences in relative bioavailability of chemicals when present in soil, indoor settled dust or water compared to the oral bioavailability corresponding with the toxicological threshold. At present, values are set at 1 by default, meaning that differences in bioavailability are not accounted for.

It is recommended not to change the values for soil and dust at the generic level if this is not supported yet by policy. You could change the values at a higher level assessment if you have site-specific information that justifies values lower than 1.

The relative bioavailability from water could be higher than 1. Changing this value is only appropriate if well-documented from toxicity and toxicodynamic studies.

4.10.4. ADJUST AGE-SPECIFIC WEIGHT FACTORS

Age-specific weight factors (for inhalation) can only be modified at Tier 2. These factors represent corrections that take into account physiological differences in children (such as the higher ventilation rate on a body weight basis) compared to adults, which could impact inhalation exposure of children. They should only be modified if you have good scientific information based on the type of toxic action. If you would have toxicological values for inhalation (Risk tab) that take into account children's sensitivity, you should consider whether the age-specific weight factors can be set at 1 for these age categories.

4.10.5. DERMAL EXPOSURE PARAMETERS

The subscreen related to dermal exposure parameters allows you to fill in the appropriate parameter values for dermal absorption from soil and dust and from water. Dermal exposure is always calculated as an absorbed dose, for which absorption values are needed.

Dermal absorption from water is calculated using a "$\mathbf{K_p}$" (dermal permeability coefficient) value. For inorganic chemicals, this is a required value. For organic chemicals, this value can be calculated by the model. In that case, you should activate the checkbox at the right of the K_p field.

Parameter	Information

Parameter	Information
K_p	• Dermal absorption from water. • Required for inorganic chemicals. • For organic chemicals, a value can be filled in or can be estimated by S-Risk; estimation is not recommended for chlorinated chemicals.
FA	• Used to calculated dermal absorption from water. • FA = 1 for inorganic chemicals. • For organic chemicals, the application domain should be checked; S-Risk calculates B and τ_{event} which can be used to check FA; if the chemical falls within the application domain, FA = 1; otherwise FA should be read from Figure 42.
ABSdermal, soil/dust	• The dermally absorbed fraction from soil or dust. • Required value.

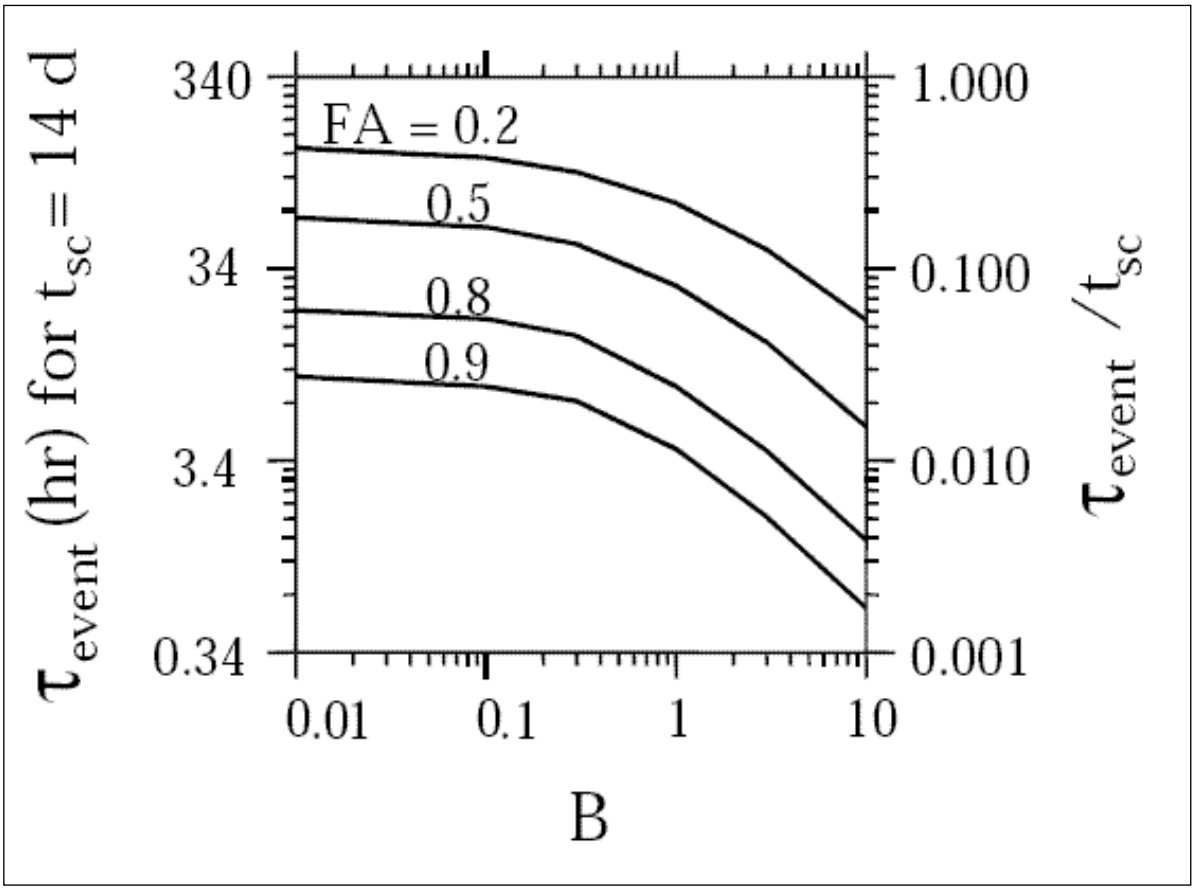


Figure 42: FA as a function of B and τ_{event} (t_{sc} equals the average turnover time of the stratum corneum and has a default value of 14 days)

4.10.6. BACKGROUND CONCENTRATIONS

Background concentrations in drinking water, outdoor air and indoor air are used to calculate background exposure.

The background concentrations in plants and animal products are only of significance in case of scenarios with consumption of local food. In that case, the concentrations are used to correct the overall dietary background exposure for the local fraction. Using the background concentrations, dietary intake is calculated for each food group and multiplied by the local fraction. This is then subtracted from the overall dietary background exposure.

4.11. RISK TAB

The Risk tab (Figure 43) allows you to modify or fill in the toxicological reference values for the substances selected. This tab is only accessible in Tier 2 when you have a modified chemical or a newly defined chemical. Risk indices and excess cancer risks are calculated for long-term exposure. The toxicological reference values should therefore correspond to long-term exposure. If short-term effects are critical, the user can take intermediate outputs of the model (daily averages, with the exception of food) and calculate short-term risks manually.

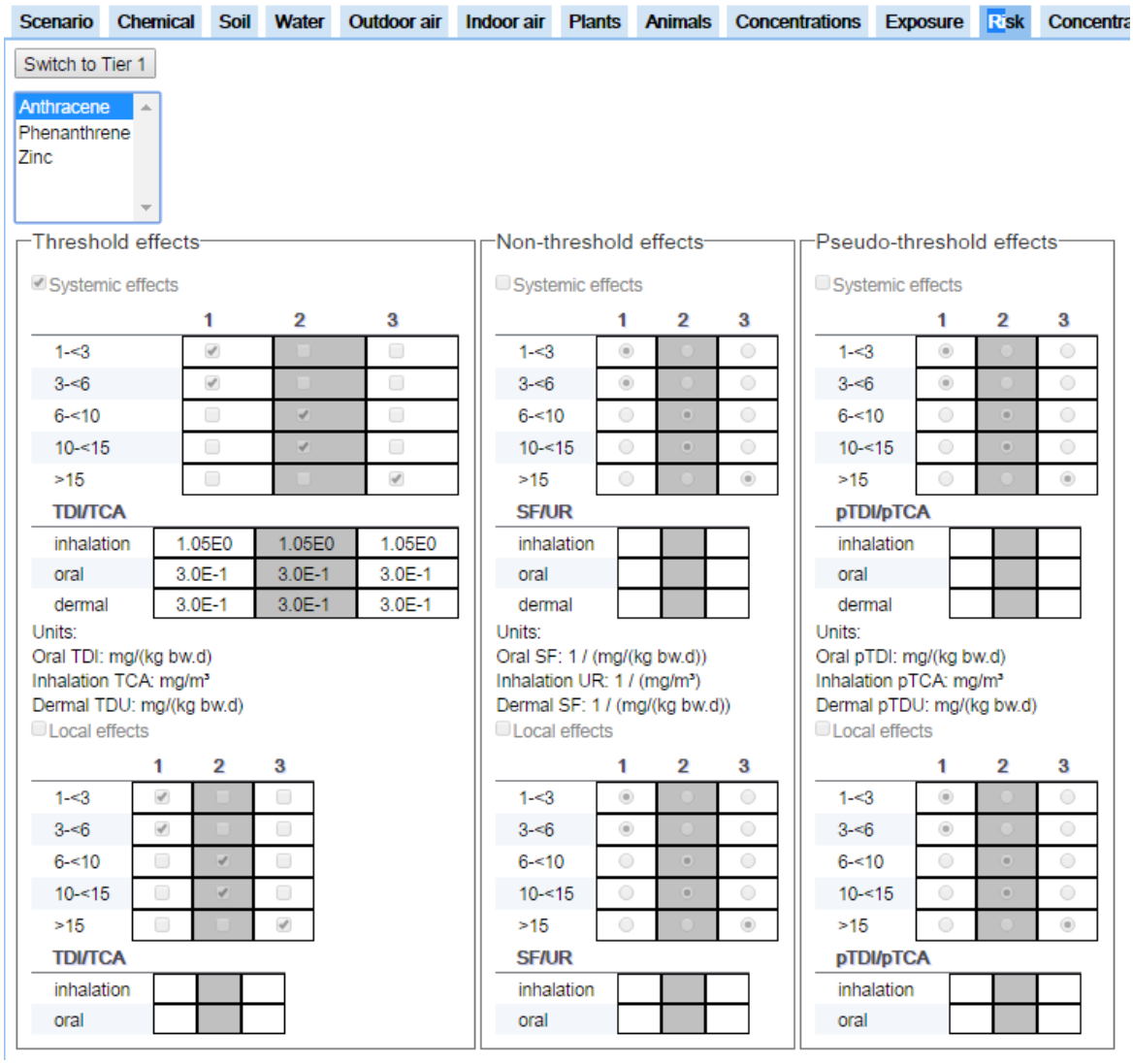


Figure 43: The risk tab in Tier 2

The tab distinguishes between three categories of effects, for which the toxicological reference values can be filled in:

- **Threshold effects**: health effects for which a threshold exists;
- **Non-threshold effects**: health effects for which no threshold exists as is the case for e.g., genotoxic carcinogens;
- **Pseudo-threshold effects**: health effects (generally carcinogenic) that cannot be classified under the two categories above. Examples are carcinogens for which no slope factor was derived, but a pseudo-threshold value; compounds such as the genotoxic carcinogen benzo(a)pyrene that has a tolerable concentration in air in the database derived from the general background (instead of using the slope factor).

For each of these three categories, two options related to the type of endpoints are available:

- **Systemic effects**: the critical endpoint is a systemic effect, meaning that the effects occur at a site in the body at a distant from the site of entry (respiratory airways, digestive tract or skin). Exposure is combined across the three routes taking into account differences in potency or bioavailability by route. *The risk index (or excess lifelong cancer risk) is calculated for each exposure route and the risk indices (or excess lifelong cancer risks) are summed to an overall risk index (or excess lifelong cancer risk);*
- **Local effects**: the critical endpoint(s) is (are) route specific. The effect occurs at the portal of entry (respiratory airways, digestive tract or skin). Exposure is not combined across the different routes. *A risk index (excess lifelong cancer risk) is calculated separately for the oral and the inhalation route*.

As chemicals sometimes have different types of health endpoints (carcinogenic and non-carcinogenic; local and systemic), it is possible to activate the options simultaneously. This enables the risk indices (or excess lifelong cancer risks) corresponding to each selection to be calculated and reported in one run. Each category and type of effect can be activated/deactivated by clicking the corresponding checkbox. Once activated, default settings for age categories and averaging will appear and can be modified by the user.

4.11.1. THRESHOLD EFFECTS

→ Systemic effects

Risk indices are calculated by route and summed up to an overall risk index. The risk index is the ratio of dose (concentration) to the toxicological reference value. A risk index above 1 is considered unacceptable under the Flemish and Brussels policy for contaminated sites. Toxicological reference values should be given for each exposure route:

- *Oral route*: TDI or Tolerable Daily Intake (mg/kg bw.d);
- *Inhalation route*: TCA or Tolerable Concentration in Air (mg/m³);
- *Dermal route*: TDU or Tolerable Daily Uptake (mg/kg bw.d); the reference value for the dermal route is an absorbed dose (as exposure for the dermal route is calculated as an absorbed dose). In many cases, a separate value for systemic effects by the dermal route is not available; a first step is to take the same value as the oral TDI. If the orally absorbed fraction is low, then the dermal TDU is calculated by multiplying the oral TDI with the orally absorbed fraction. More refined estimates can be required in case of route-specific metabolism.

There are three age classes for which a risk index can be calculated. By default the age classes are set as follows:

- Age class 1: 1 – < 3 yr; 3 - < 6 yr;
- Age class 2: 6 - < 10 yr; 10 - < 15 yr;
- Age class 3: > 15 yr.

This can be modified if the risk index should be calculated for a different range of ages by clicking the check boxes in the age class / age ranges table. A condition is set that within an age class, the ages selected should be continuous. In addition to specifying the age range per age class, it is possible to specify the toxicological reference values for age class 1, 2 or 3 by filling in the fields below each age class. In general, no differentiation will be made between age classes, but if age-differentiated reference values are available, they can be used. It should be noted that the calculation of the inhalation risk already considers age-dependent factors weighting the concentrations (based on dosimetry) as can be accessed through the Exposure tab under the age-specific weight factors. Age-dependent differences in the Risk tab for all routes should therefore generally reflect potency or bioavailability differences and not intake differences. It could therefore be advisable to evaluate the age-dependent weight factors and the toxicological reference values together for the inhalation route.

→ **Local effects**

Risk indices are calculated for the oral and inhalation route. It is not possible to have a risk index calculated for local effects by the dermal route, as the dermal dose is calculated as an absorbed dose in the model. If local dermal effects are critical, the user should perform additional calculations outside S-Risk by using intermediate results. Toxicological reference values for local effects should be given in for the oral and/or inhalation route (depending on whether local effects occur by both or only one route).

Options for age classes and the type of toxicological reference values (oral/inhalation) are the same as under Systemic effects.

4.11.2. NON-THRESHOLD EFFECTS

→ **Systemic effects**

Excess lifelong cancer risks are calculated by route and summed up to an overall excess lifelong cancer risk. The lifelong cancer risk is calculated by multiplying the dose (concentration) with the slope factor (unit risk). A lifelong cancer risk above $1/10^5$ is considered unacceptable under the Flemish and Brussels policy on contaminated sites. Toxicological reference values should be given for each exposure route:

- *Oral route*: SF or Slope Factor $((mg/kg\ bw.d)^{-1})$;
- *Inhalation route*: UR or Unit Risk $((mg/m^3)^{-1})$;
- *Dermal route*: dermal SF or Slope Factor $((mg/kg\ bw.d)^{-1})$. The reference value for the dermal route is a slope factor related to absorbed doses (as exposure for the dermal route is calculated as an absorbed dose). In many cases a separate value for systemic effects by the dermal route is not available; a first step is to take the same value as the oral SF. If the orally absorbed fraction is low, then the dermal SF is calculated by dividing the oral SF by

the orally absorbed fraction. More refined estimates can be required in case of route-specific metabolism.

The lifelong cancer risk is calculated by averaging over all age classes. It is possible to specify slope factors/ unit risks for three age classes (1, 2 and 3). This is done by selecting the appropriate age ranges for each age class in the age class/age ranges table. Age ranges should be continuous within one age class. In general, no differentiation in slope factors/unit risks will be made between age classes (all age ranges assigned to age class 1, except if one wants to see the results by age category), but if age-differentiated reference values are available, they can be used. If more than one age class is defined, the excess cancer risk will be shown for these age classes and for lifelong exposure. It should be noted that the calculation of inhalation risk already considers age-dependent factors weighting the concentrations (based on dosimetry) as can be accessed through the Exposure tab under the age-specific weight factors. Age-dependent differences in the Risk tab for all routes should therefore generally reflect potency and bioavailaibility differences and not intake differences. It could therefore be advisable to evaluate the age-dependent weight factors and the toxicological reference values together for the inhalation route.

→ **Local effects**

Excess lifelong cancer risks are calculated for the oral and inhalation route. It is not possible to have a cancer risk calculated for local effects by the dermal route, as the dermal dose is calculated as an absorbed dose in the model. If local dermal effects are critical, the user should perform additional calculations outside S-Risk by using intermediate results. Toxicological reference values for local effects should be given for the oral and/or inhalation route (depending on whether local effects occur by both or only one route).

Options for age classes and the type of toxicological reference values (oral/inhalation) are the same as under Systemic effects.

4.11.3. PSEUDO-THRESHOLD EFFECTS

→ **Systemic effects**

Pseudo-risk indices are calculated by route and summed up to an overall pseudo-risk index. The pseudo-risk index is the ratio of dose (concentration) to the toxicological reference value. A pseudo-risk index above 1 is considered unacceptable under the Flemish and Brussels policy for contaminated sites. As pseudo-threshold effects mainly relate to carcinogens, a lifelong risk index is calculated. Toxicological reference values should be given for each exposure route:

- *Oral route*: pTDI or pseudo-Tolerable Daily Intake (mg/kg bw.d);
- *Inhalation route*: pTCA or pseudo-Tolerable Concentration in Air (mg/m³);
- *Dermal route*: pTDU or pseudo-Tolerable Daily Uptake (mg/kg bw.d). The reference value for the dermal route is an absorbed dose (as exposure for the dermal route is calculated as an absorbed dose). In many cases, a separate value for systemic effects by the dermal route is not available; a first step is to take the same value as the oral pTDI. If the orally absorbed fraction is low, then the dermal pTDU is calculated by multiplying the oral pTDI with the orally absorbed fraction. More refined estimates can be required in case of route-specific metabolism.

The lifelong pseudo-risk index is calculated by averaging over all age classes. It is possible to specify toxicological reference values for three age classes (1, 2 and 3). This is done by selecting the appropriate age ranges for each age class in the age class/age ranges table. Age ranges should be continuous within one age class. In general, no differentiation will be made between age classes (all age ranges assigned to age class 1, except if one wants to see the results by age category), but if age-differentiated reference values are available, they can be used. If more than one age class is defined, the lifelong pseudo-risk will be shown for these age classes and for lifelong exposure. It should be noted that the calculation of inhalation risk already considers age-dependent factors weighting the concentrations (based on dosimetry) as can be accessed through the Exposure tab under the age-specific weight factors. Age-dependent differences in the Risk tab for all routes should therefore generally reflect potency and bioavailability differences and not intake differences. It could therefore be advisable to evaluate the age-dependent weight factors and the toxicological reference values together for the inhalation route.

→ **Local effects**

Lifelong pseudo risk indices are calculated for the oral and inhalation route. It is not possible to have a risk index calculated for local effects by the dermal route, as the dermal dose is calculated as an absorbed dose in the model. If local dermal effects are critical, the user should perform additional calculations outside S-Risk by using intermediate results. Toxicological reference values for local effects should be given in for the oral and/or inhalation route (depending on whether local effects occur by both or only one route).

Options for age classes and the type of toxicological reference values (oral/inhalation) are the same as under pseudo-threshold - systemic effects.

4.11.4. DEFAULT CHOICE

In the absence of more specific information, the default choice is as follows:

- Threshold effects – systemic effects (in case of non-carcinogens or carcinogens with a threshold for effects):
  - Age classes: *1* (1 – < 3 yr; 3 - < 6 yr); *2* (6 - < 10 yr; 10 - < 15 yr); *3* (> 15 yr);
  - TDI/TCA values are the same for each age class ;
  - Dermal TDU is the same as the oral TDI;
- Non-threshold effects – systemic effects (in case of carcinogens with no threshold for effects):
  - Age classes: 1 (1 – < 3; 3 - < 6); 2 (6 - < 10; 10 - < 15); 3 (> 15);
  - Oral SF/inhalation UR values are the same for each age class;
  - Dermal SF is the same as the oral SF.

4.12. CONCENTRATION LIMITS TAB

The values in the Concentration limits tab are only accessible in Tier 2 and in case of a newly defined or customized chemical. In case of a default chemical or in Tier 1, the values are only visible (Figure 44). To fill in values, select the chemical for which you want to enter or modify values and go to the appropriate fields. The Concentration limits tab allows you to enter (legal) concentration limits for which predicted or measured concentrations in transfer media are compared with.

It is not required to fill in limits for all fields, fields can be left empty if there are no values.

For plant concentration limits, it is possible to enter limits at the level of the plant or to group plants and enter a limit at group level. The groups are marked by grey/white colouring. If you would like to enter a limit value at group level, you can activate one of the checkboxes of that plant group. The other checkboxes of that group will be activated after pressing <Enter>. You can then fill in the limit for either field of that plant group and after pressing <Enter>, the value will automatically be copied to the other fields of that plant group.

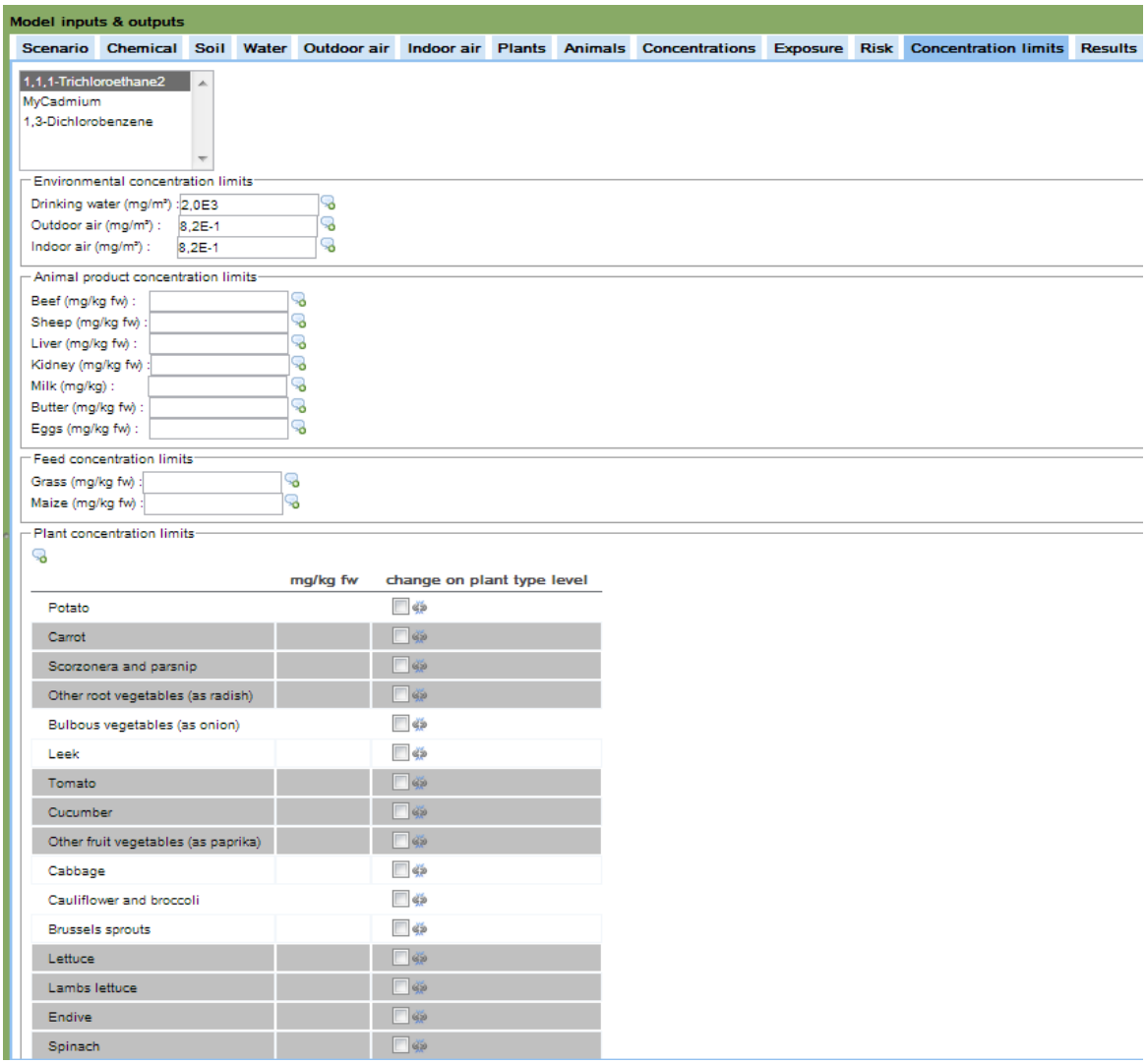


Figure 44: Concentration limits tab (at Tier 2)

4.13. RESULTS TAB

After entering the input parameter values for your simulation, calculations will be possible. You can start calculations by clicking the "**Calculate risks & report results**" button on the Results tab (Figure 45).

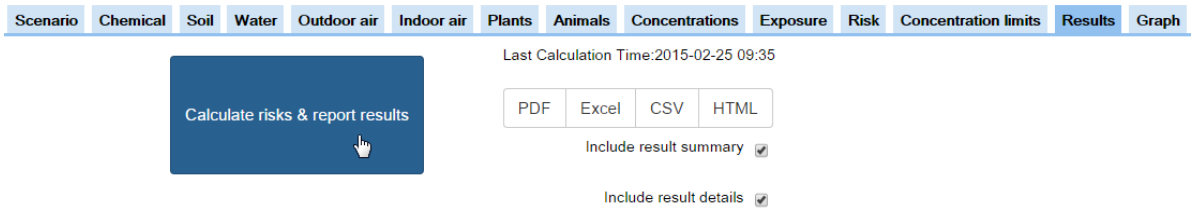


Figure 45: Starting calculations on the Results tab

After clicking the button, a dialog will appear mentioning that calculations have started. After clicking OK on this dialog, the colour of your simulation in the "Available simulations" panel turns yellow, indicating that calculations are running (Figure 46).

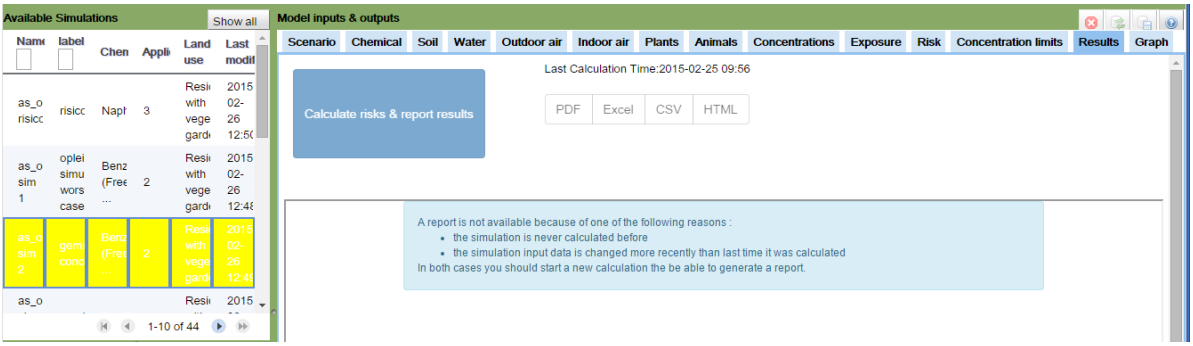


Figure 46: Yellow colouring indicating the simulation is running

When simulation calculations are finished, you will receive a message that the simulation calculations are completed successfully. If – for any reason – the calculation would be unsuccessful, the simulation will be marked red in the "Available simulations" panel.

Simulation calculations are run on one of our calculation servers, so you can close your browser during calculations. If you would lose internet connection during the calculations, there is no problem as calculations will simply continue running on our calculation servers. You will be able to access your results after your internet connection has been restored.

After a successful run, you will be able to download the results of your most recent simulation on the Results tab (Figure 47), by clicking the button of the report format of your choice. The simulation report is available in PDF, Excel, CSV and HTML formats and can be downloaded to store for later use.

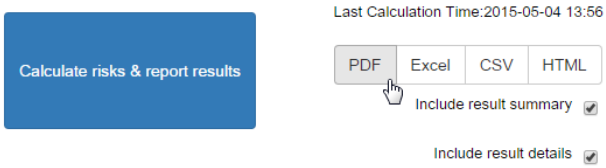


Figure 47: Simulation results downloadable from Results tab

You can customize the extended report to include “result summary” and/or “result details” sections in the report. The result summary includes the main risk index and concentration index results and a summary of exposure results per pathway. The result details section adds further detailed intermediary calculation and exposure results. In any case, every report generated is intended to be complete so that it is possible to exactly reproduce calculations based on the report (it is not possible to download a report with the simulation input values only).

Besides downloading result reports, you can also consult an online result summary of your simulations (Figure 48). When this report doesn’t show automatically, you can click on the link provided on the *Results* tab, which refers you directly to the HTML page of this report. An overview of the highest RI, ExCR, pRI and/or CI calculated per chemical can be found in the Main results section. Information with regard to the chosen land use type, considered exposure routes (these are labelled and marked in green), site characteristics, added soil layers and concentrations is summarized in the Conceptual site model section. Next, results per chemical (i.e., risk indexes, concentration indexes, an exposure overview and local vs. background exposure) are shown. An overview of the parameters you have modified in your simulation, can be consulted in the List of user-modified parameters section. Lastly, the S-Risk versions in which you have created and calculated your simulation can be found on the bottom of the online result summary. The region for which you are currently logged in, is shown here as well. If you would like to print this summary, you can click on the blue Print button above the Main results section. By using the report outline on the right, you can quickly go to the section of your interest.

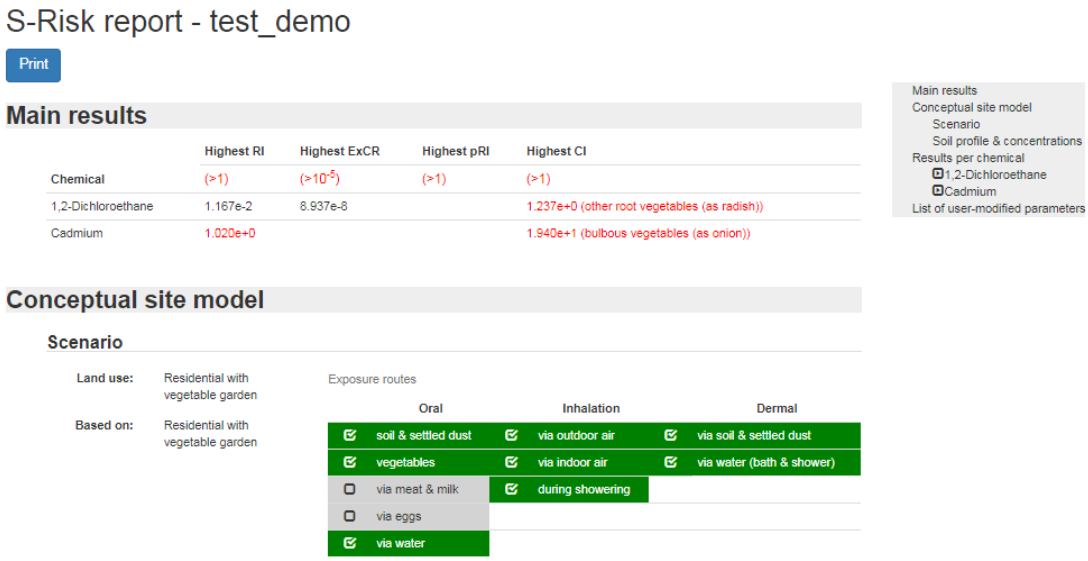


Figure 48: Online result summary on Results tab

4.14. GRAPH TAB

The graph tab enables the S-Risk user to visualize the influence of pollutant concentrations in a specific soil/groundwater layer on a specific risk or concentration index. This visual feedback provides more context on the risk calculations for a specific simulation configuration. Figure 49 shows this graphing interface.

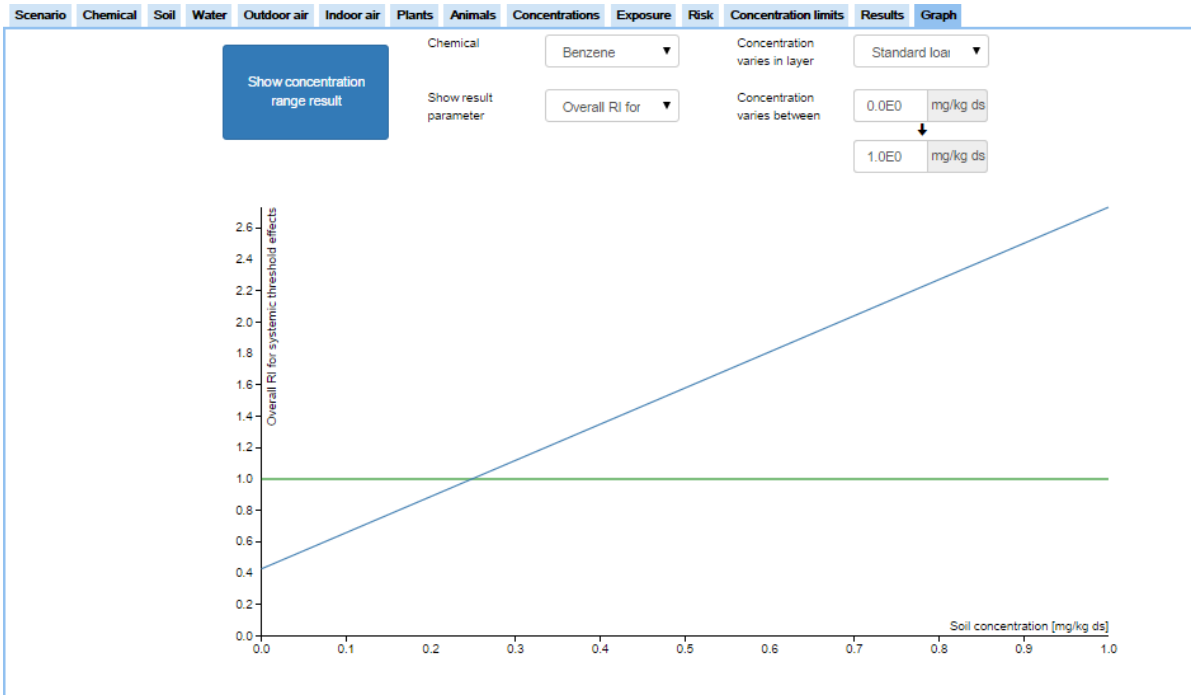
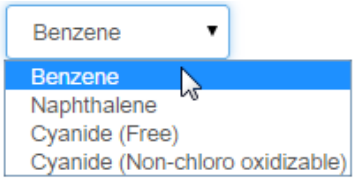


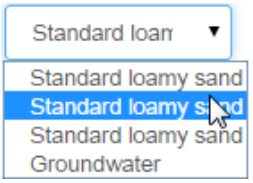
Figure 49: The Graph tab interface

You can use the Graph tab functionality by following these steps:

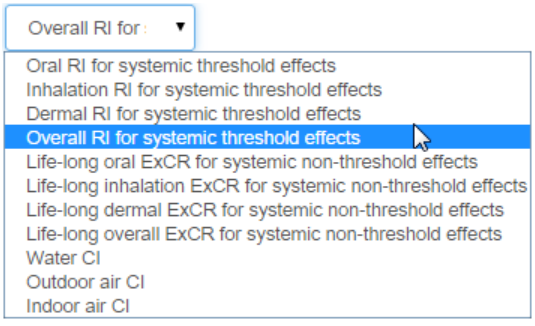
1. Select the chemical for which you want to visualize the risks in the "Chemical" menu.



2. Choose the soil/groundwater layer for which you want to vary the concentration. This determines the X axis of the graph.



3. Select the risk or concentration index parameter that you want to visualize. This determines the Y axis of the graph.



4. Specify the concentration range that you want to visualize. S-Risk will visualize the chosen result parameter over this range.

5. Click the “Show concentration range result” button to start the calculations.

You will be informed by the browser when calculations start, and when they have finished. Afterwards, a graph will be shown visualizing the result parameters’ evolution, given the concentration range you have specified.

If the “Show concentration range result” button is disabled (“greyed out”), this usually means that some input information (steps 1 – 4) is still missing.

This graphing functionality allows the user to:

- quickly get an overview of how the risk evolves in function of the concentration, without the need to manually change concentrations;
- quickly estimate remediation goals by visualizing the point where, for example, the risk index exceeds the RI = 1 level;
- get more context for the results in Application I and III.

The green line in the Graph tab represents the cut-off value (CI=1 or (p)RI=1 or ExCR=1x10^{-5}). The blue line represents the actual progress of the risk or concentration index in function of increasing soil concentration.

CHAPTER 5 APPLICATION III SIMULATIONS

When you choose application type III simulations, remediation objectives will be calculated for the layer that you specify. You can fill in the data for your simulation exactly the same way as you do for an application II simulation (forward calculation). The only difference is on the "**Concentrations**" and "**Results**" tab.

5.1. CONCENTRATIONS TAB

In case of an application III, you need to specify the layer for which you want the optimization (calculation of remediation objective) to be run for. This option is available at the bottom of the Concentrations tab (Figure 50). This can be a soil layer or, if you have chosen to have an entered groundwater concentration, the groundwater layer. If you have chosen to have the groundwater concentration being calculated, you cannot optimize on groundwater concentration.

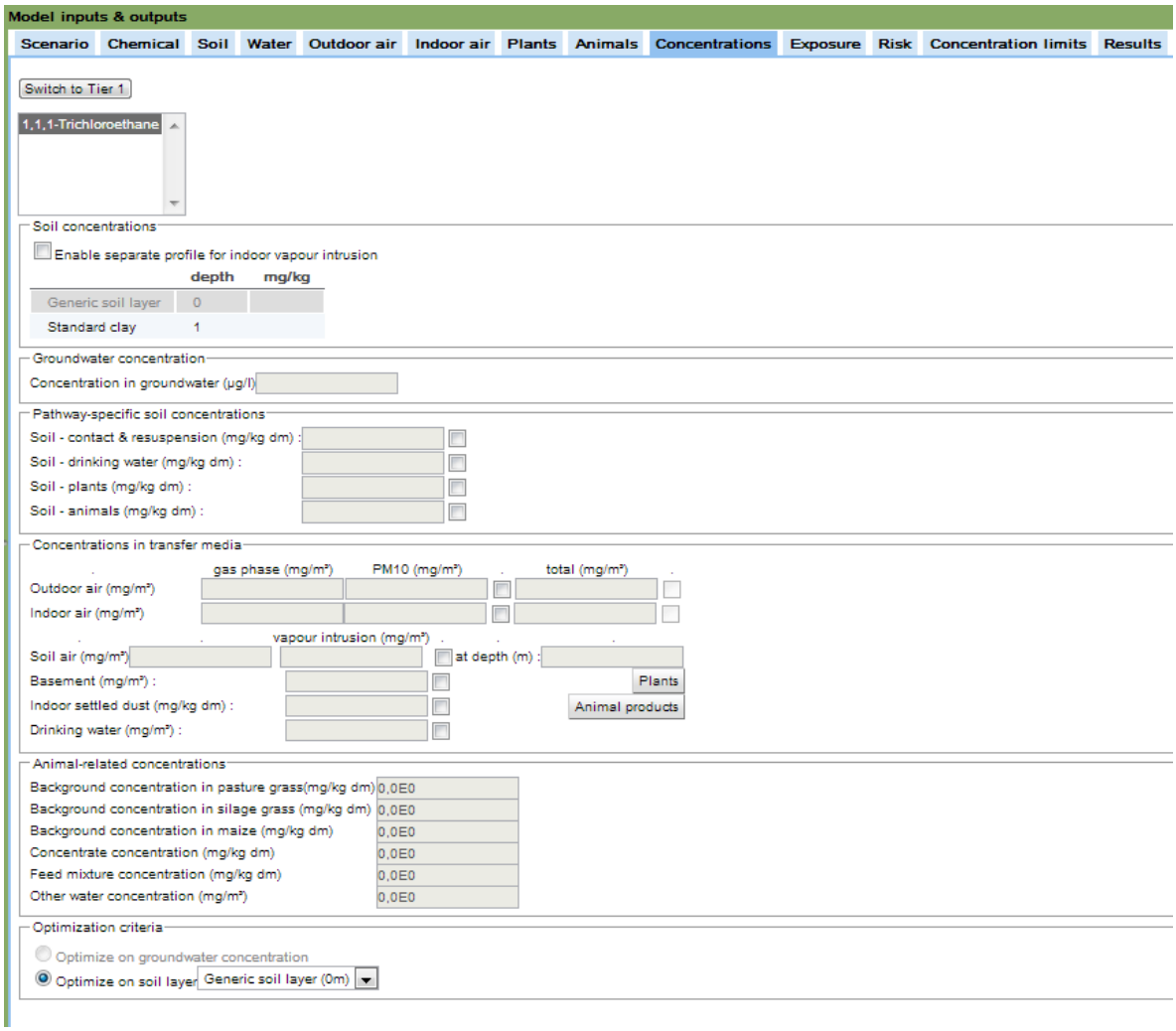


Figure 50: Concentrations tab for an application III simulation (Tier 2)

Once you select the layer for which you want to optimize, the field allowing you to enter concentrations ("**Soil concentrations**" subscreen) will be disabled for that layer. You will still be able (required) to fill in concentrations for the other soil layers and, if appropriate, for the groundwater layer. Filled in concentrations will be kept constant during optimization and only the exposures linked to the layer selected for optimization will vary (between 0 and 10^6 mg/kg dm for soil layers and between 0 and 10^9 µg/L for groundwater) until the optimization procedure is finalized.

The Concentrations tab still allows you to fill in "**pathway-specific soil concentrations**" and "**concentrations in transfer media**". We recommend to consider these vary carefully in case of application III simulations. If concentrations are filled in here, the pathway calculations will not change during optimization (i.e., the concentrations or exposures will remain constant), which could give undesirable results.

5.2. RESULTS TAB

After entering the data for your simulation, calculations will be possible. You can start calculations by clicking the "**Calculate remediation objectives & report results**" button on the Results tab, similar to what you do under Application II.

The report will now not generate risks or concentration indices, but will for each specified criterion report the concentration at which the criterion is met. The criterions are:

- Exposure and threshold effects or pseudo-threshold effects: the risk index equals 1 (or the ratio of total exposure to tolerable intake equals 1);
- Exposure and non-threshold effects: the excess cancer risk equals $1/10^5$;
- Concentrations in transfer media: the concentration index equals 1 (or the ratio between concentration and concentration limit equals 1).

Just as under Application II, you can consult an online result summary and detailed report of your simulation in Application III. Only here, the Main results section of the online result summary gives an overview of the lowest RI-, ExCR-, pRI- and/or CI-based remediation value calculated per chemical, the Conceptual site model section shows you for which layer the optimization was done (i.e., the concentrations for that layer are indicated as "(Optimized)") and the Results per chemical section provides now information about risk- and CI-based remediation values.

The optimization procedure only considers *realistic* ranges of soil or groundwater concentrations:

- soil concentrations: 0 – 10^6 mg/kg dm;
- groundwater concentrations: 0 – 10^9 µg/L.

Automatic optimization algorithms are never perfect, so in a number of situations S-Risk will not find a critical concentration within the range mentioned, or find a possibly incorrect critical concentration. In all cases, these situations will be clearly indicated in the report.

A small overview of these situations:

1. The risks associated with the pollutant in the optimized layer are very low, and consequently, none of the concentrations in the range 0-10^6 mg/kg dm (or 0-10^9 µg/L for groundwater) causes risks exceeding the limit value. The critical concentration is set to 10^6 mg/kg dm for soil layers or to 10^9 µg/L for groundwater;

2. The layer to be optimized always involves a risk (e.g., due to high background exposure), or another layer than the optimized one is determining the risk. Consequently, none of the concentrations in the range 0-10^6 mg/kg dm (or 0-10^9 µg/L for groundwater) results in a value lower than the limit value. The critical concentration is set to 0 for both soil and groundwater;
3. The chemical substance (i.e., Cu, Ni, Hg, Zn or Pb) uses non-standard models resulting in discontinuities or a non-monotonous behavior of the relation between soil/groundwater concentration and RI/pRI/ExCR/CI. Mathematically speaking, there are multiple possible solutions for the critical soil concentration, and the critical concentration found can be misleading. For this type of situation, it is recommended to check the optimization result by using the Graph tab;
4. An unforeseen error did occur (e.g., certain input data were not provided resulting in a failure to calculate the critical concentration ("empty" result)). For this type of situation, it is recommended to check the input data provided, to check the optimization result by using the Graph tab and/or to contact the helpdesk.

For all situations described above, S-Risk will give clear warning messages in both the online result summary (the number of the footnote behind the critical concentration corresponds with the numbers described above) and the detailed report.

CHAPTER 6 APPLICATION I SIMULATIONS

Application I is a restricted version of application III and allows you to calculated generic soil remediation values or risk limit values.

6.1. SCENARIO TAB

Under application I, it is only possible to select a land use from the default land use list. It is not possible to customize land uses. You can view the default settings.

6.2. CHEMICAL TAB

You can select chemicals, customize them or add a new chemical as explained under application II (Chemical tab).

6.3. SOIL TAB

You can remove the default generic soil type and add a soil type from the list of soil types. You can only have one soil layer. The groundwater table is at a fixed depth (of 3 m). You can change organic matter content, clay content and pH-KCl at Tier 1 and customize the soil type at Tier 2 (see also description of Soil tab under application II).

6.4. WATER, OUTDOOR AIR, AND INDOOR AIR TAB

These tabs can be consulted, but not be modified.

6.5. PLANTS, ANIMALS, CONCENTRATIONS, EXPOSURE, RISK AND CONCENTRATION LIMITS TAB

These tabs only have editable fields in case of a customized or newly added chemical.

6.6. RESULTS TAB

After entering the data for your simulation, calculations will be possible. You can start calculations by clicking the "**Calculate and report results**" button on the Results tab, similar to what you do under Application II.

The report will now not generate risks or concentration indices, but will for each specified reference value report the soil concentration at which the criterion is met. The criterions are:

- Exposure and threshold effects or pseudo-threshold effects: the risk index equals 1 (or the ratio of total exposure to tolerable intake equals 1);
- Exposure and non-threshold effects: the excess cancer risk equals $1/10^5$;

- Concentrations in transfer media: the concentration index equals 1 (or the ratio between concentration and concentration limit equals 1).

Just as under Application II, you can consult an online result summary of your simulation in Application I. Only here, the Main results section gives an overview of the lowest RI-, ExCR-, pRI- and/or CI-based remediation value calculated per chemical, the Conceptual site model section shows you for which layer the optimization was done (i.e., the concentrations for that layer are indicated as "(Optimized)") and the Results per chemical section provides now information about risk- and CI-based remediation values.

The optimization procedure only considers *realistic* ranges of soil or groundwater concentrations:

- soil concentrations: 0 – 10^6 mg/kg dm;
- groundwater concentrations: 0 – 10^9 µg/L.

Automatic optimization algorithms are never perfect, so in a number of situations S-Risk will not find a critical concentration within the range mentioned, or find a possibly incorrect critical concentration. In all cases, these situations will be clearly indicated in the report.

1. A small overview of these situations:The risks associated with the pollutant in the optimized layer are very low, and consequently, none of the concentrations in the range 0-10^6 mg/kg dm causes risks exceeding the limit value. The critical concentration is set to 10^6 mg/kg dm;
2. The soil layer to be optimized always involves a risk (e.g., due to high background exposure) , or another layer than the optimized one is determining the risk. Consequently, none of the concentrations in the range 0-10^6 mg/kg dm results with a value lower than the limit value. The critical concentration is set to 0;
3. The chemical substance (i.e., Cu, Ni, Hg, Zn or Pb) uses non-standard models resulting in discontinuities or a non-monotonous behavior of the relation between soil concentration and RI/pRI/ExCR/CI. For this type of situation, it is recommended to check the optimization result by using the Graph tab;
4. An unforeseen error did occur (e.g., certain input data were not provided resulting in a failure to calculate the critical concentration ("empty" result)). For this type of situation, it is recommended to check the input data provided, to check the optimization result by using the Graph tab and/or to contact the helpdesk.

For all situations described above, S-Risk will give clear warning messages in both the online result summary (the number of the footnote behind the critical concentration corresponds with the numbers described above) and the detailed report.

6.7. GRAPH TAB

Also under Application I, you can use the Graph tab to visualize the influence of pollutant concentrations in a specific soil/groundwater layer on a specific risk or concentration index. The steps you have to follow to do this, are the same as explained under Application II.