**EXTERNAL SCIENTIFIC REPORT**

# User manual to the software tool (PERSAM) for calculating predicted environmental concentrations (PECs) of plant protection products (PPPs) in soil for annual crops

CFT/EFSA/PRAS/2012/03

**Lieve Decorte, Ingeborg Joris, Stijn Van Looy, Jan Bronders**

VITO

## ABSTRACT

The software application Persistence in Soil Analytical Model (PERSAM) assists the user in performing calculations using the analytic model, as described in the Opinion. More specifically, the software tool will be able to calculate: TIER-1 PEC's, TIER-2B 95$^{th}$-percentile PEC's, TIER-2C 95$^{th}$-percentile PEC's using output from TIER-2A simulations with numerical models for the soil load including wash-off, and to select the grid cell including the scenario properties corresponding to the 95$^{th}$-percentile PEC as needed for the scenario development of TIER-3



## KEY WORDS

exposure assessment, soil, plant protection products, soil organisms, ecotoxicological effects, tiered approaches, crop interception, Help file, Persistence in Soil Analytical Model (PERSAM), PERSAM

## DISCLAIMER



Any enquiries related to this output should be addressed to pesticides.ppr@efsa.europa.eu

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## SUMMARY

In EFSA, the Pesticides Unit and the Panel on Plant Protection Products and their Residues are responsible for the risk assessment of pesticides. The activities of the Pesticides Unit are related to: (i) the risk assessment of pesticides, including the development of risk assessment methodologies; (ii) peer review of the safety of active substances used in plant protection products in the EU; (iii) risk assessment in the framework of setting Maximum Residue Levels (MRLs), the permitted upper legal levels of pesticide residues in food and/or feed at the EU level; (iv) compilation and analysis of the monitoring information on pesticide residues generated in EU Member States (including some EFTA countries), assessment of the actual consumer exposure to pesticide residues and recommendations for future pesticide monitoring activities at the European level.

The aims and objectives of the project are to develop a software tool for calculating the predicted environmental concentrations of substances and their transformation products in soil in support of the EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. The tool will be based on an analytical model for which both the concepts and the mathematical equations are described in the Scientific Opinion, (EFSA, 2012b).

The software application assist the user in performing calculations using the analytic model, as described in the opinion. More specifically, the software tool will be able to calculate:

- ✓ TIER-1 Predicted Environmental concentrations
- ✓ TIER-2B 95$^{th}$-percentile PEC's
- ✓ TIER-2C 95$^{th}$-percentile PEC's using output from TIER-2A simulations with numerical models for the soil load including wash-off, and
- ✓ To select the grid cell including the scenario properties corresponding to the 95$^{th}$-percentile PEC as needed for the scenario development of TIER-3

The project started in December 2012 and was finalised in April 2014.
This document contains the user manual of Persistence in Soil Analytical Model (PERSAM) version 1.0.

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## BACKGROUND AS PROVIDED BY EFSA

In EFSA, the Pesticides Unit and the Panel on Plant Protection Products and their Residues are responsible for the risk assessment of pesticides. The activities of the Pesticides Unit are related to: (i) the risk assessment of pesticides, including the development of risk assessment methodologies; (ii) peer review of the safety of active substances used in plant protection products in the EU; (iii) risk assessment in the framework of setting Maximum Residue Levels (MRLs), the permitted upper legal levels of pesticide residues in food and/or feed at the EU level; (iv) compilation and analysis of the monitoring information on pesticide residues generated in EU Member States (including some EFTA countries), assessment of the actual consumer exposure to pesticide residues and recommendations for future pesticide monitoring activities at the European level.

A number of Member States expressed interest in a revision of the current SANCO Guidance Document on persistence in soil (SANCO/9188VI/1997 of 12 July 2000) during the general consultation of Member States on Guidance Documents in answer to the request by EFSA sent *via* the Standing Committee on the Food Chain and Animal Health. Furthermore the previous PRAPeR Unit (now Pesticides Unit) noted that the existing SANCO Guidance Document (SANCO/9188VI/1997 of 12 July 2000) needs to be updated.

Besides the development of an EFSA Guidance Document for predicting environmental concentrations of plant protection products (PPPs) in soil, software tools need to be developed to calculate the exposure of PPPs in soil. The computerized tools will be released for use by applicants and risk assessors for the evaluation of PPPs and transformation products according to Parliament and Council Regulation (EC) 1107/2009.

The modelling tools to be developed together with the EFSA guidance document, should allow a consistent, reliable and science-based exposure assessment in soil for the evaluation of PPPs and their transformation products under Regulation (EC) 1107/2009.

## TERMS OF REFERENCE AS PROVIDED BY EFSA

This contract was awarded by EFSA to:

VITO

Contract title: Development of software models for predicting environmental concentrations of plant protection products in soil

Contract number: CTF/EFSA/PRAS/2012/03

## 1. Introduction

In EFSA, the Pesticides Unit and the Panel on Plant Protection Products and their Residues are responsible for the risk assessment of pesticides. The activities of the Pesticides Unit are related to: (i) the risk assessment of pesticides, including the development of risk assessment methodologies; (ii) peer review of the safety of active substances used in plant protection products in the EU; (iii) risk assessment in the framework of setting Maximum Residue Levels (MRLs), the permitted upper legal levels of pesticide residues in food and/or feed at the EU level; (iv) compilation and analysis of the monitoring information on pesticide residues generated in EU Member States (including some EFTA countries), assessment of the actual consumer exposure to pesticide residues and recommendations for future pesticide monitoring activities at the European level.

The software tool Persistence in Soil Analytical Model (PERSAM) is developed for calculating the predicted environmental concentrations of substances and their transformation products in soil in support of the EFSA guidance document for predicting environmental concentrations of PPP's in soil. The tool will be based on an analytical model for which both the concepts and the mathematical equations are described in the Scientific Opinion.(Question number: EFSA-Q-2011-00282, EFSA Journal 2012;10(2):2562 [76 pp.]. doi:10.2903/j.efsa.2012.2562 )

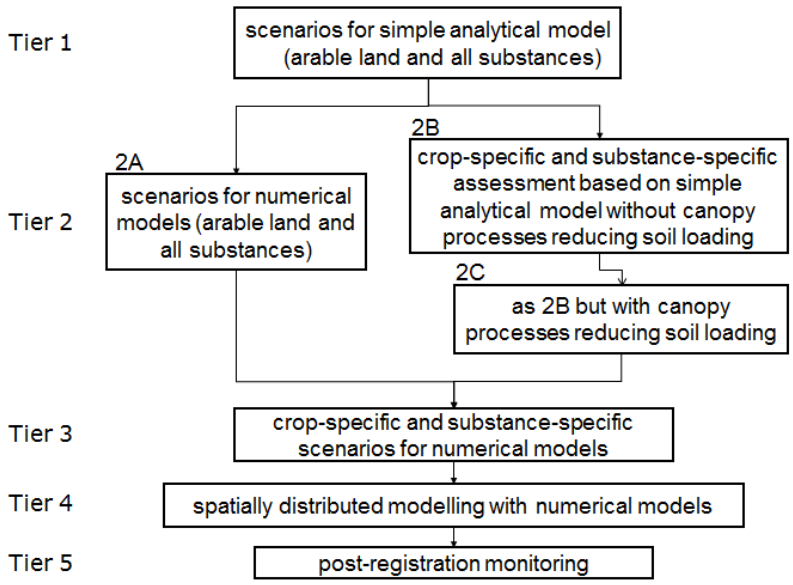



**Figure 1: EFSA, 2015 in prep. EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil**

The software application assist the user in performing calculations using the analytic model, as described in the opinion. More specifically, the software tool performs calculations for:

- ✓ TIER-1 PEC's
- ✓ TIER-2B 95th-percentile PEC's
- ✓ TIER-2C 95th-percentile PEC's using output from TIER-2A simulations with numerical models for the soil load including wash-off, and
- ✓ To select the grid cell including the scenario properties corresponding to the 95th-

percentile PEC as needed for the scenario development of TIER-3

## 2. Tutorial

Use the Tutorial for a quick start with the application.



### ***How can you start the PERSAM application?***

1. Start your browser and go to the JRC soil portal

   http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/
2. Install the PERSAM application
3. Go to your start menu
4. Select the application PERSAM

   If you cannot find the application, then you have to go to start menu/programs


**Figure 2: PERSAM - Startup screen**

***How can you create a group?***

1. Right mouse click in the left pane of the Welcome window
2. Select 'New group'
3. Give a group name
4. Click on 'Create'

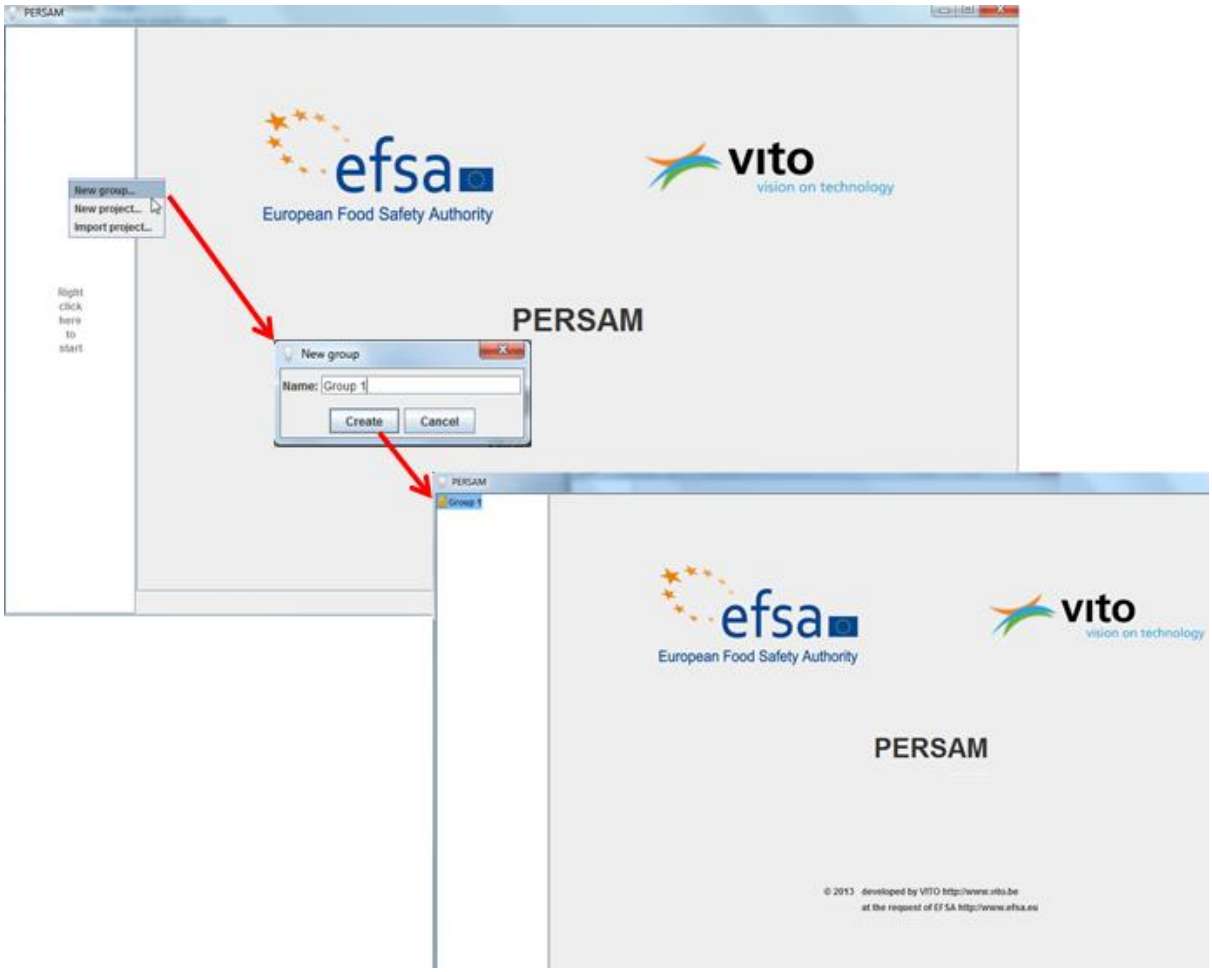



**Figure 3:Project management - Create a new group**

***How can you create a project?***

1. Select first the group and right mouse click
2. Select 'New project'
3. Give a project name
4. Click on 'Create'
5. Give a project description

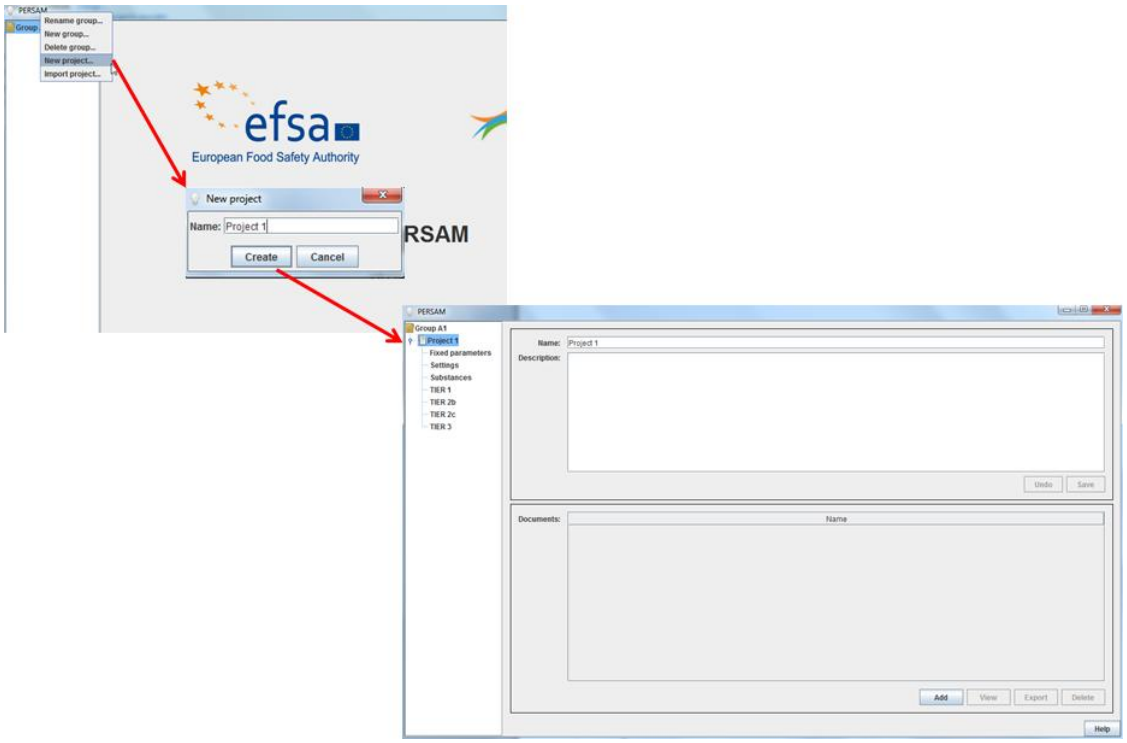



**Figure 4:Project management - Create a new project**

***How can you view the fixed parameters of the project?***

1. Go to the project tree
2. Select 'Fixed parameters'

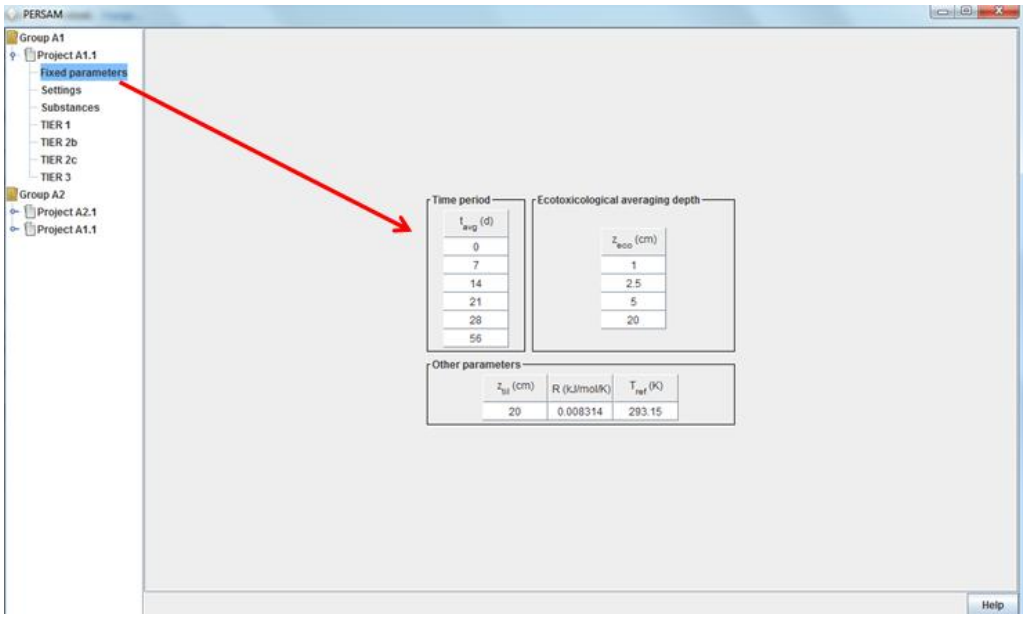



**Figure 5:Fixed parameters**

***How can you change the settings for the project?***

1. Go to the project tree
2. Select 'Settings'
3. Select both endpoints 'concentration in liquid phase' and 'concentration in total soil'
4. Select a CAPRI crop (e.g. Maize) and click on 'Save'

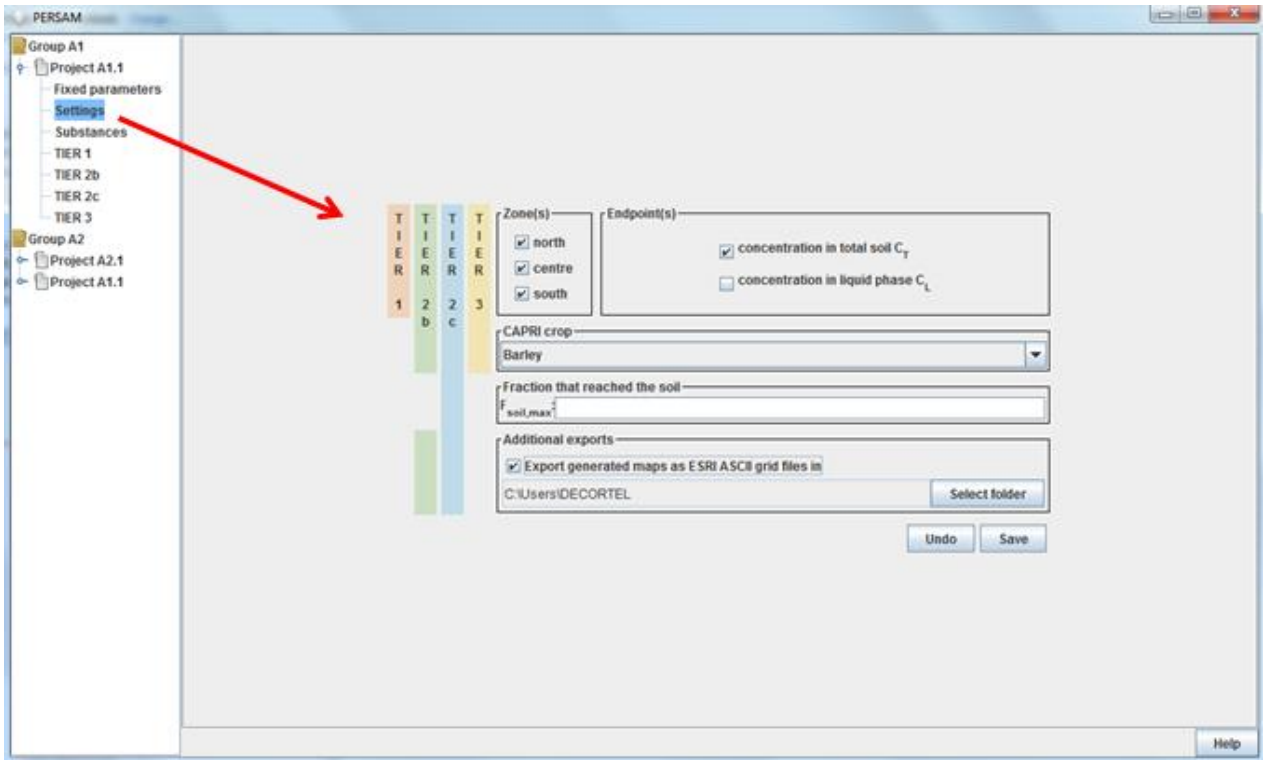



**Figure 6: Settings section**

***How can you define a parent substance?***

1. Go to the project tree and select 'Substances'
2. Click on a place holder in the tree and the screen 'Configure substance' appears.
3. Select one of the build in substances in the drop down list (e.g. standard substance 1)
4. The screen shows automatically the related parameters of the selected substance.These parameters are not editable.
5. Click 'OK'
6. Define the Time between applications and the annual application rate of the active substance.
7. Click 'Save'

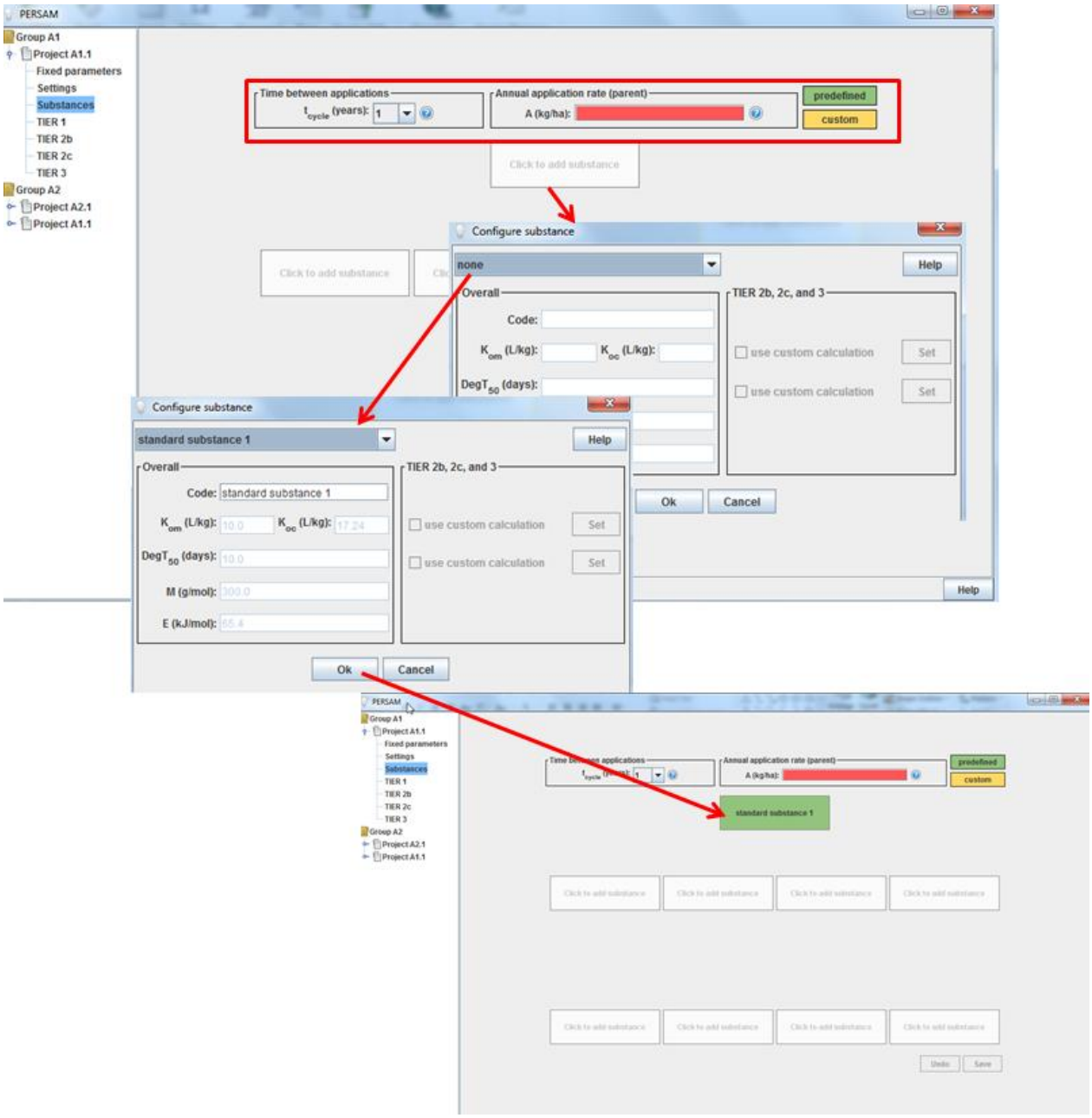



**Figure 7:Configure a predefined substance (parent or metabolite)**

## ***How can you define metabolites?***

1. Go to the project tree and select 'Substances'
2. Click on a place holder in the tree and the screen 'Configure substance' appears.
3. Select one of the build in substances in the drop down list (e.g. standard substance 2)
4. The screen shows automatically the related parameters of the selected substance.These

parameters are not editable.

5. Click 'OK'

***Additional information***

- Define customized substances or metabolites: see *Configure custom substance*
- Define custom calculations for Kom or for DegT50 based on spatial parameters or on pH dependent sorption: see *Configure custom calculations*

***How can you define the relationship between the parent substance and a metabolite?***

Links are represented as arrows between the place holders in the tree structure.

1. Click on an arrow between two place holders that contain a substance and the dialog 'Configure link' appears. The source and target substance fields are informative: they cannot be changed.

2. Enable the checkbox 'Link enabled'.
   Unchecking the' link enabled' checkbox will disable an arrow (grey), keeping it enabled will enable the arrow (black).

3. Define the formation factor

4. Click 'OK'

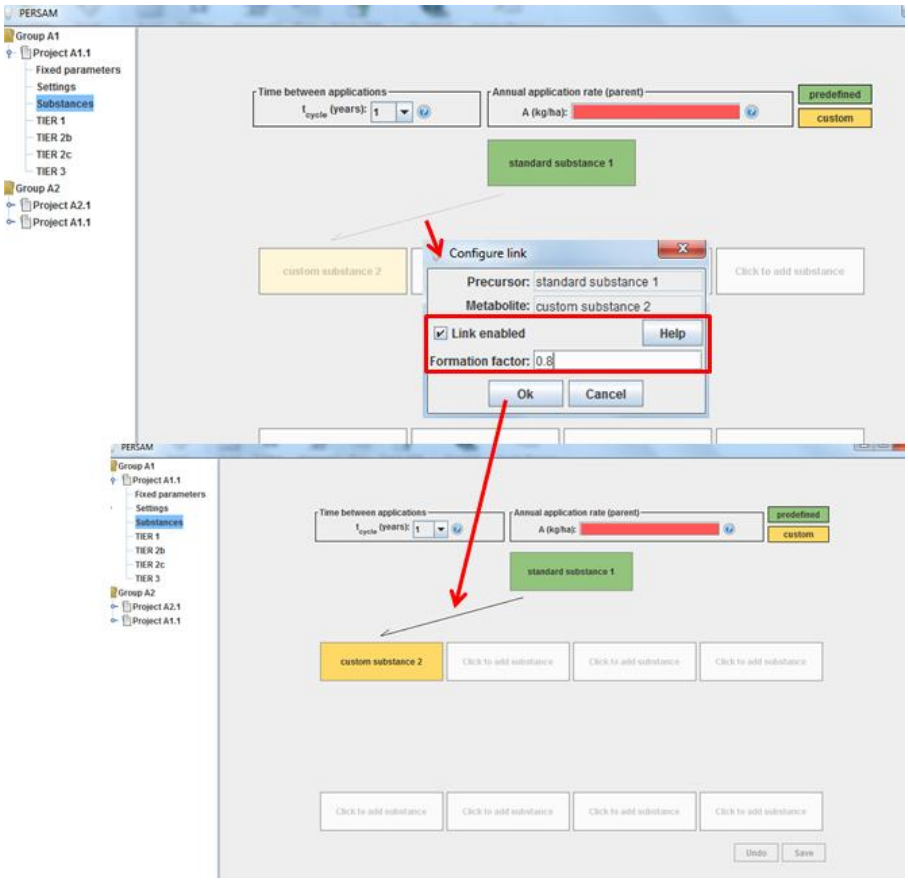



**Figure 8:Configure a link**

***How can you perform the TIER-1 calculations?***

1. Go to the project tree and select 'TIER-1'
2. Select the result tab.
3. Click on 'Start' and the calculations start.
4. The results appear on the screen. Select a substance in the Substance tree to view the results.

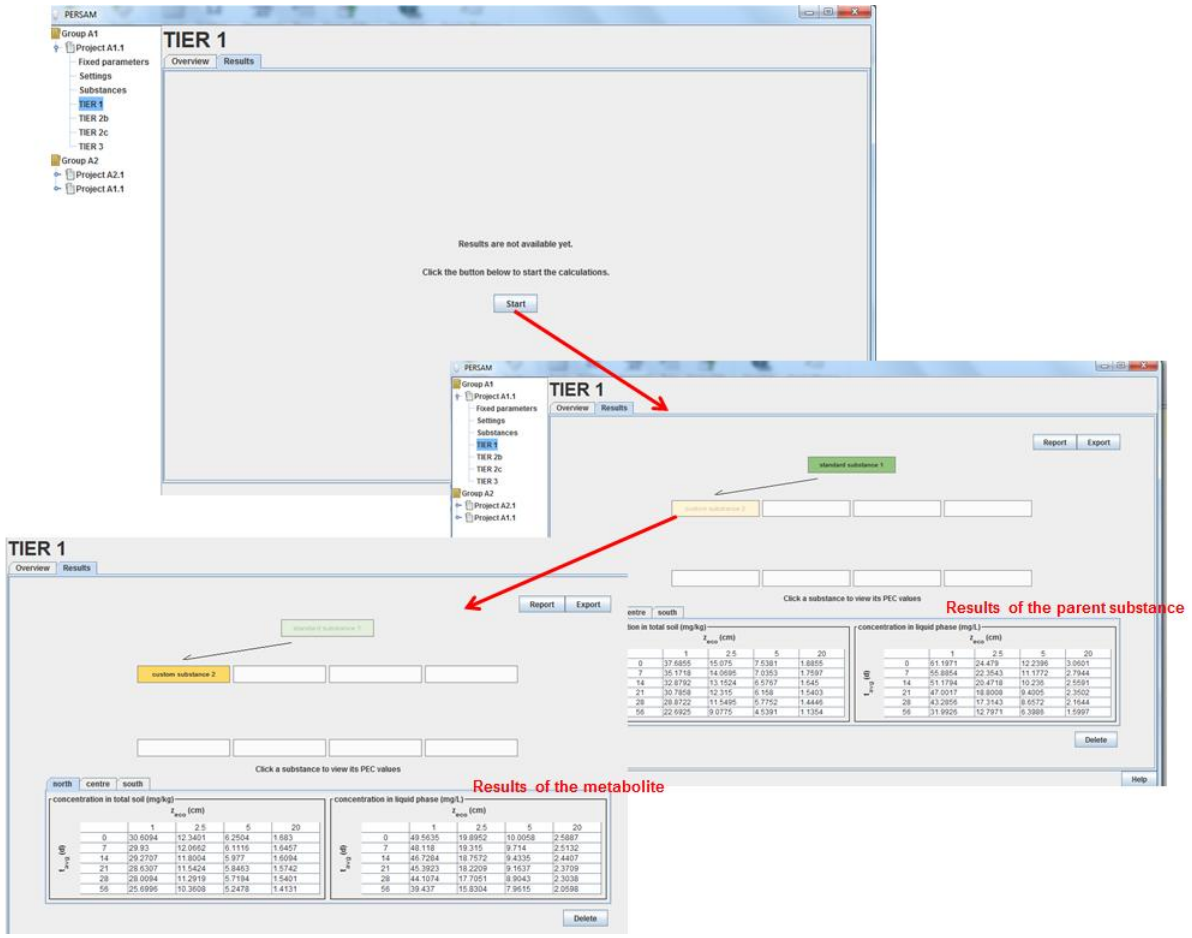



**Figure 9:Results of TIER-1**

***How can you perform the TIER-2B calculations?***

1. Go to the project tree and select 'TIER-2B'
2. Select the result tab.
3. Click on 'Start' and the calculations start.
4. The results appear on the screen. Select a substance in the Substance tree to view the results. The table contains a field for each combination of endpoint, ecotoxicological averaging depth and time window.
5. Click on a cell in the table to view extended results. A detail window appears containing the 95$^{th}$ spatial percentile of calculated PECs for the regulatory selected zone with the related cumulative distribution graph and map.

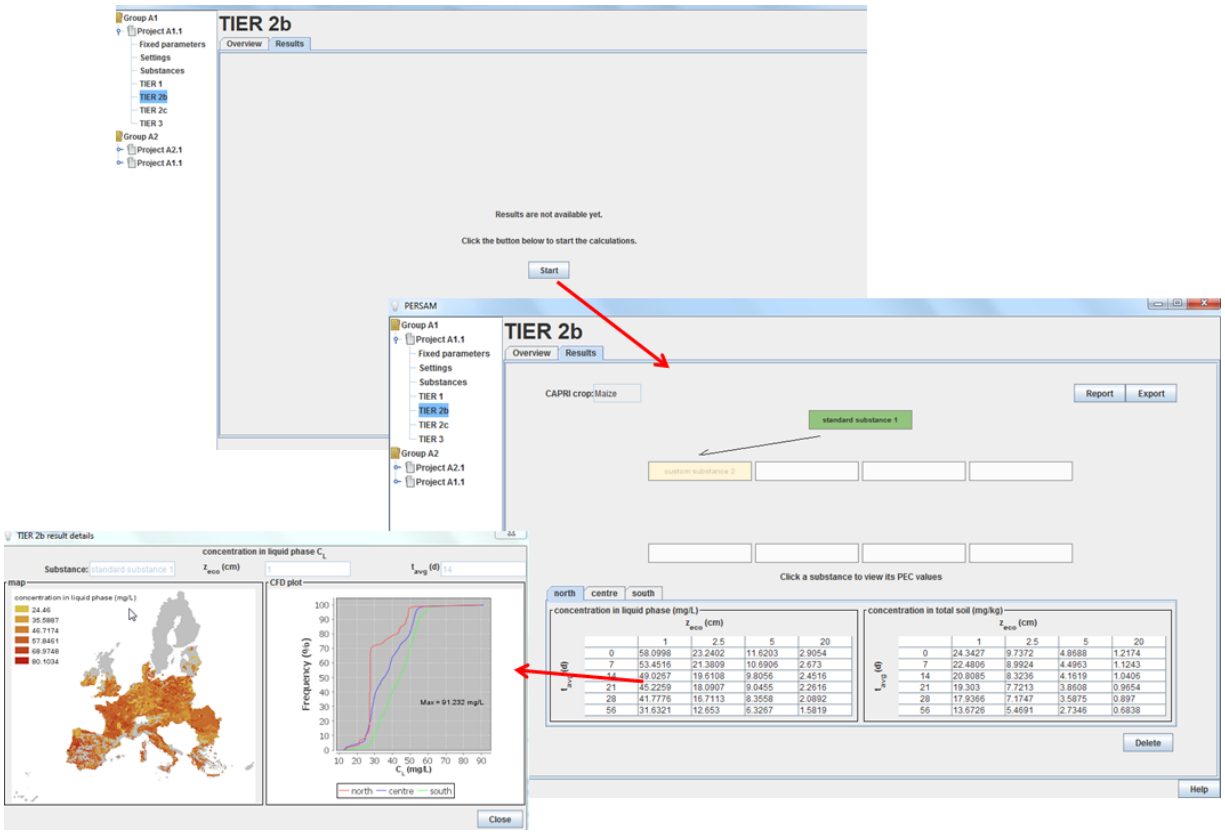



**Figure 10: Results of TIER-2B**

***How can you perform the TIER-2C calculations?***

1. Go to the project tree and select 'Setting'
2. Define the fraction that reaches the soil $F_{soil,max}$
3. Go to the project tree and select 'TIER-2C'
4. Select the result tab.
5. Click on 'Start' and the calculations start.
6. The results appear on the screen. Select a substance in the Substance tree to view the results. The table contains a field for each combination of endpoint, ecotoxicological averaging depth and time window.
7. Click on a cell in the table to view extended results. A detail window appears containing the 95$^{th}$ spatial percentile of calculated PECs for the regulatory selected zone with the related cumulative distribution graph and map.

***How can you perform the TIER-3 calculations?***

1. Go to the project tree and select 'TIER-3'
2. Go to the 'Results' tab
3. Select a substance in the Substance tree to view the results. The results tab of TIER-3 contains a table with the green cells which indicates whether there results are available
4. Click on a particular cell (a combination of ecotoxicological averaging depth, time window and endpoint) and there will appear a result window containing the model parameters for the TIER-3 scenario and the vulnerability map showing the calculated vulnerability indices and the location of the grid cell corresponding to a 95% vulnerability.

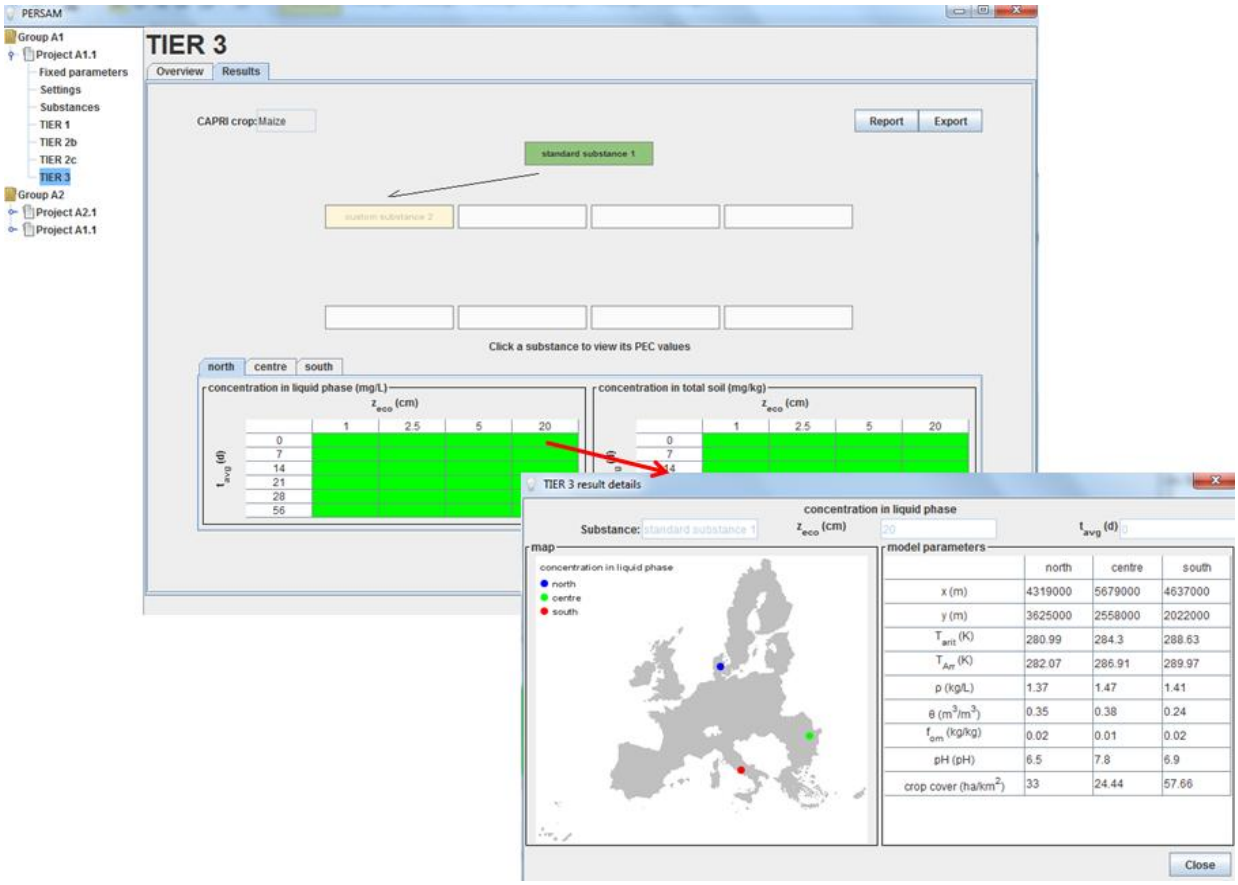



**Figure 11: Results of TIER-3**

***How can you create a PDF report of the TIER-3 parameters?***

1. On the results tab of TIER-3, click on 'Report'
2. The popup window 'Generate report' appears. Give the location where you want to save the PDF report
3. Click on 'Save'
   PERSAM generates and opens the PDF report.

**Remark:** You can use the information of the PDF report in other WORD documents, by selecting the text in the PDF report and copy/paste to the word document.

***Tips*:**

- Before you install a new version of PERSAM, export all your projects. After the installation you can import the projects so that you don't lose any data.
- You can delete a substance in the substace tree by clicking on a configured substance and selecting the value 'Non' in the drop down list of the popup window 'Configure substance'.
- You can remove a relationship between substances by clicking on the link and uncheck the 'link enabled' checkbox. The arrow will be disabled (gray).
- If you need PERSAM information in word documents, create first a PDF report and select the PERSAM information. Copy the selected text and paste it into your word document.
- Define always the Time between applications and the annual application rate, before you go to the calculations.

# 3. Installation

Installation of the PERSAM requires no additional licensed software tools or applications.The software is down-loadable and will automatically be installed on your pc.
For more information go to the JRC soil portal (*http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/)*
The software requires 1.2GB disk space for the installation. It is advisable to provide 10 GB of free disk space to comfortably work with PERSAM for the sake of the required temporary disk space.

Installation procedure

1. Start your browser and go to the JRC soil portal
   (*http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/)*
2. Download the software:

   → Save the software on your computer and start the installation from your computer by double click on the executable

   or

   → Start immediately the installation

3. If you have already PERSAM installed on your computer, you will get next message:

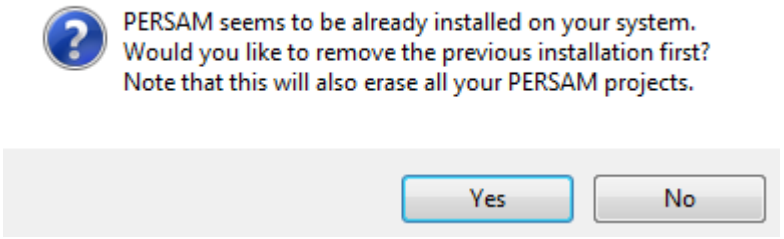



**Figure 12: Message 'PERSAM already installed'**

   → Yes: all PERSAM projects will be erased

   → No: the installation won't start and you can export the PERSAM projects and import the projects after the installation.

4. Starting the installation procedure

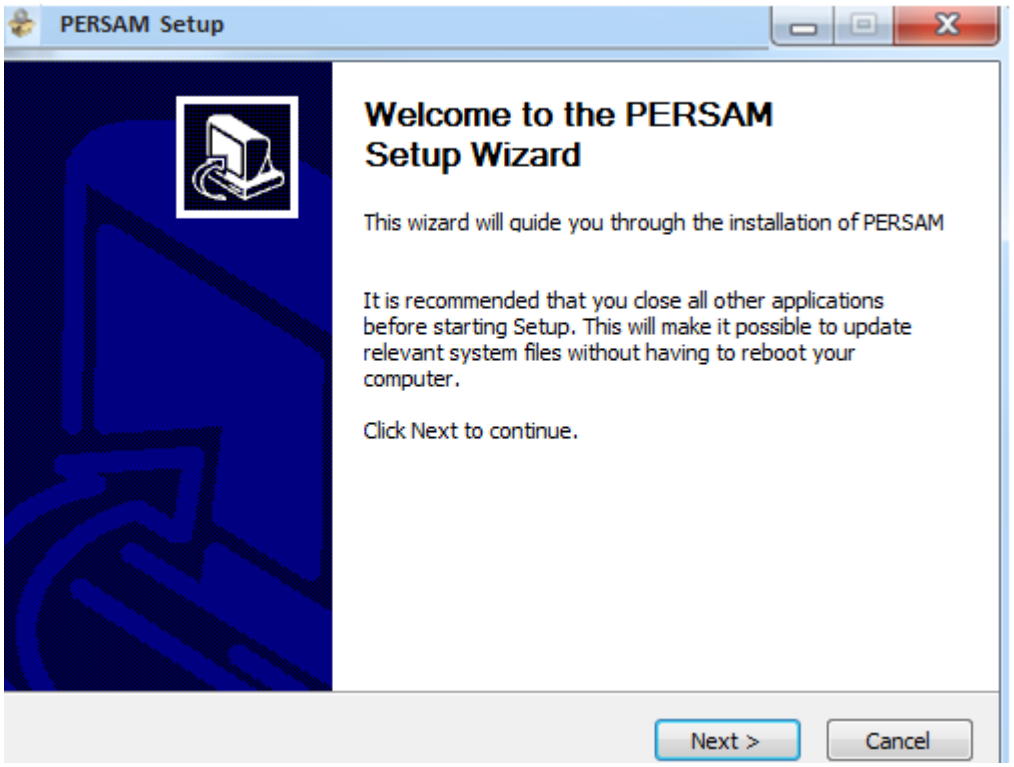



**Figure 13: Installation procedure - Welcome screen**

→ Click on 'Next'

→ The license agreement appears and click on 'I agree'

→ Choose the installation directory:

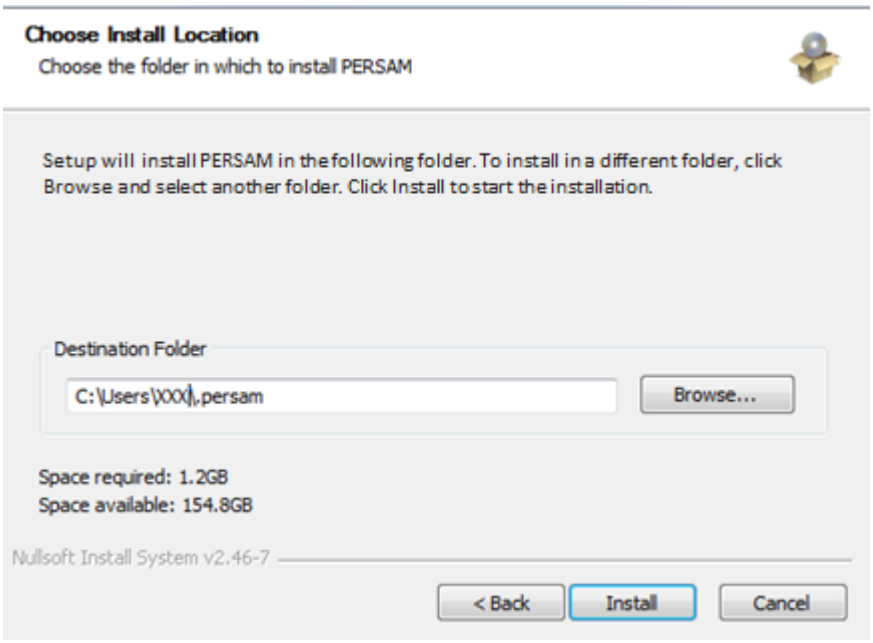



**Figure 14: Installation procedure - Choose installation directory**

→ Select the destination folder and click on 'Install'

→ The installation will start

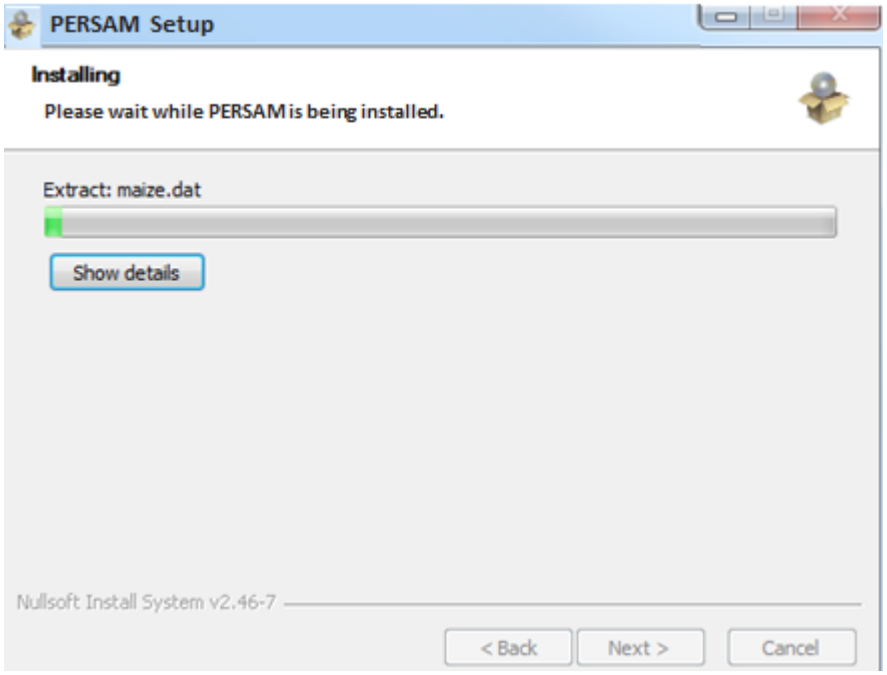



**Figure 15: Installation procedure - Installing the software**

→ After the installation, click on 'Finish'

5. You can find the PERSAM application in the start menu of your computer:

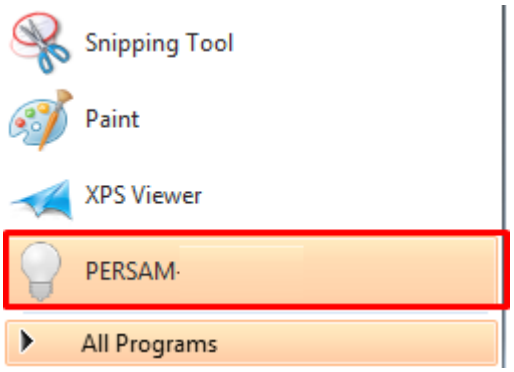



**Figure 16: PERSAM application in start menu**

### 3.1. System requirements

PERSAM is a stand-alone application running on Windows XP, Windows 7, and Windows 8, Windows 2008 server and later. For previous versions of windows not supported by Microsoft, we cannot guarantee that the software application will run on these versions. The software tool can be installed on a server so that users can use the application using remote desktop VNC software.

The software application is freely down-loadable, for more information go to the EFSA-website (*http://www.efsa.europa.eu/*). The installation of the software tool will not require additional software tools or applications, and should be by a self contained installation package (auto-installing).
The software requires 1.2GB disk space for the installation. It is advisable to provide 10 GB of free disk space to comfortably work with PERSAM for the sake of the required temporary disk space.

### 3.2. Maps

The software application incorporates EFSA spatial data set version 1.1, available on the JRC-website. (http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/) Incorporation of new map data, available from the JRC website, is possible and results into a new version of the software tool.

For more additional information: see http://eusoils.jrc.ec.europa.eu/library/Data/EFSA

### 3.3. Licensing

The software application don't uses third party libraries subjected to license agreement constraints.

### 3.4. Version number

The current version number is visible in the general window of PERSAM.


**Figure 17: Where can you find the current version number of PERSAM?**

## 4. Project management

The user input is organized in projects. A project bundles the user input for a single set of the different PEC calculation methods and the results of those calculations.

Projects can be organized freely by the user in a tree structure similar to a file system: directories (called 'group' in the tool) which can contain other directories and files (the projects in the tool)

- Group operations:
  - Create a new group
  - Modify an existing group (rename)
  - Delete a group

- Project operations:
  - Define a new project:
    - an empty project
    - from a previously exported project (import a project)
    - from a copied project (from clipboard)
  - Open an existing project
  - Modify and save a project
  - Export a project:
    - to a file
    - to clipboard (copy)
  - Delete a project

Project management with the tree structure for organizing the projects is located at the left side of the screen.

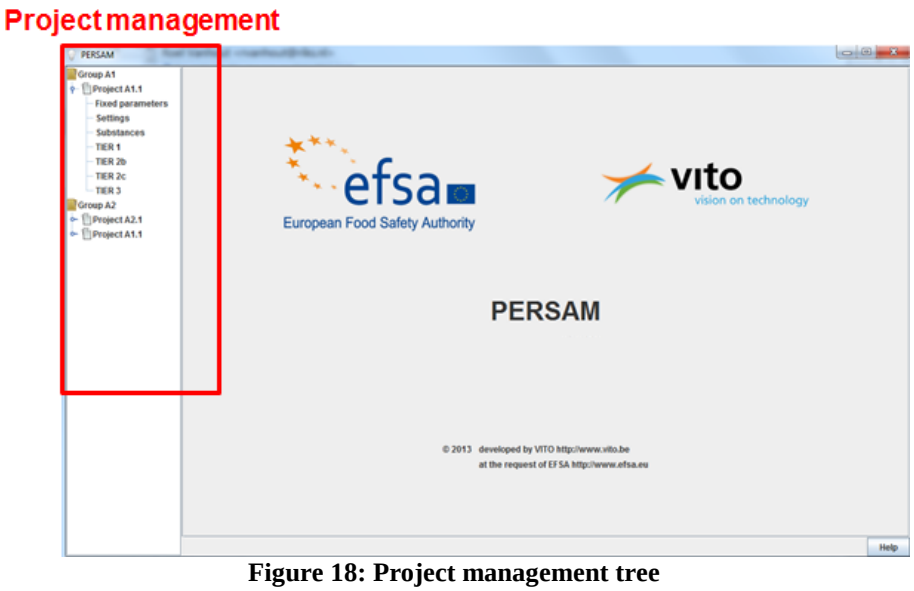



**Figure 18: Project management tree**

## 4.1. Group

A group is a collection of one or more projects in the tree structure.

**Related functionalities**:

- New group
- Rename group
- Delete group

### 4.1.1. New group

The user creates a new group.

1. Right mouse click in the left pane of the Welcome window
2. Select 'New group'
3. Give a group name
4. Click on 'Create'

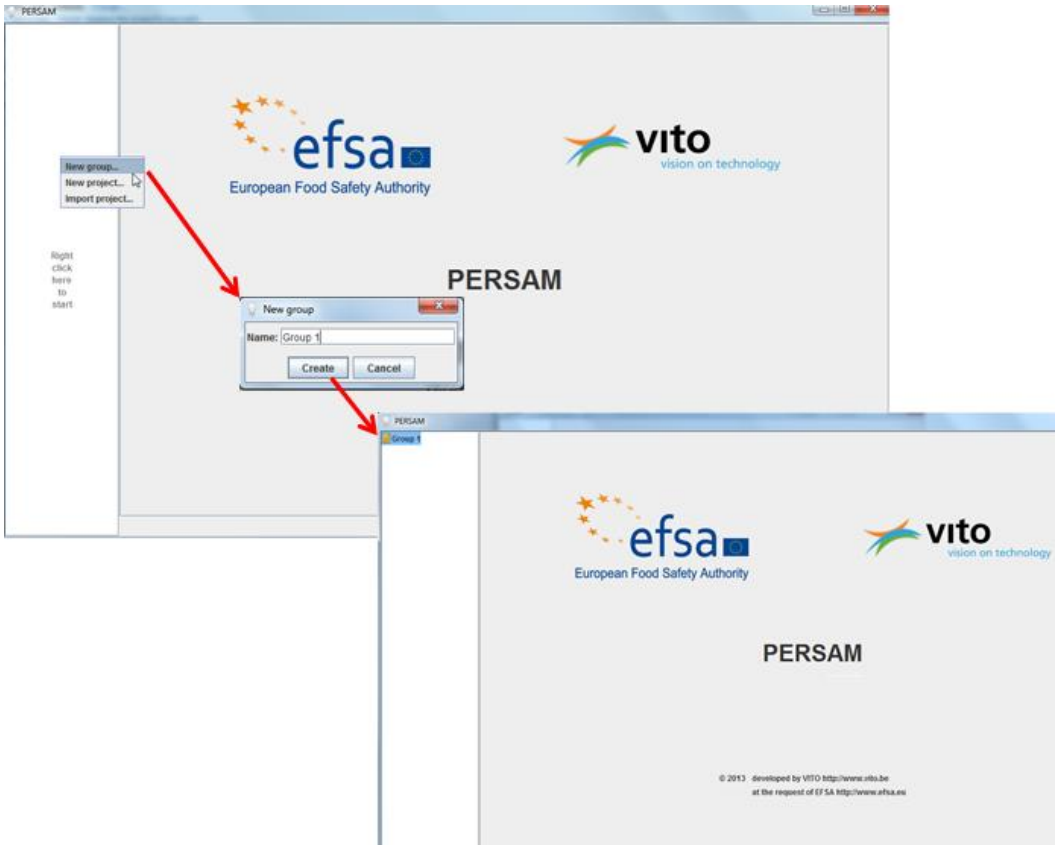


**Figure 19: New group**

### 4.1.2. Rename group

The user can give another name to an existing group.

1. Select a group
2. Right mouse click and select 'Rename group', while you keep the cursor on the selected group.
3. Give a new name
4. Click on 'Rename'

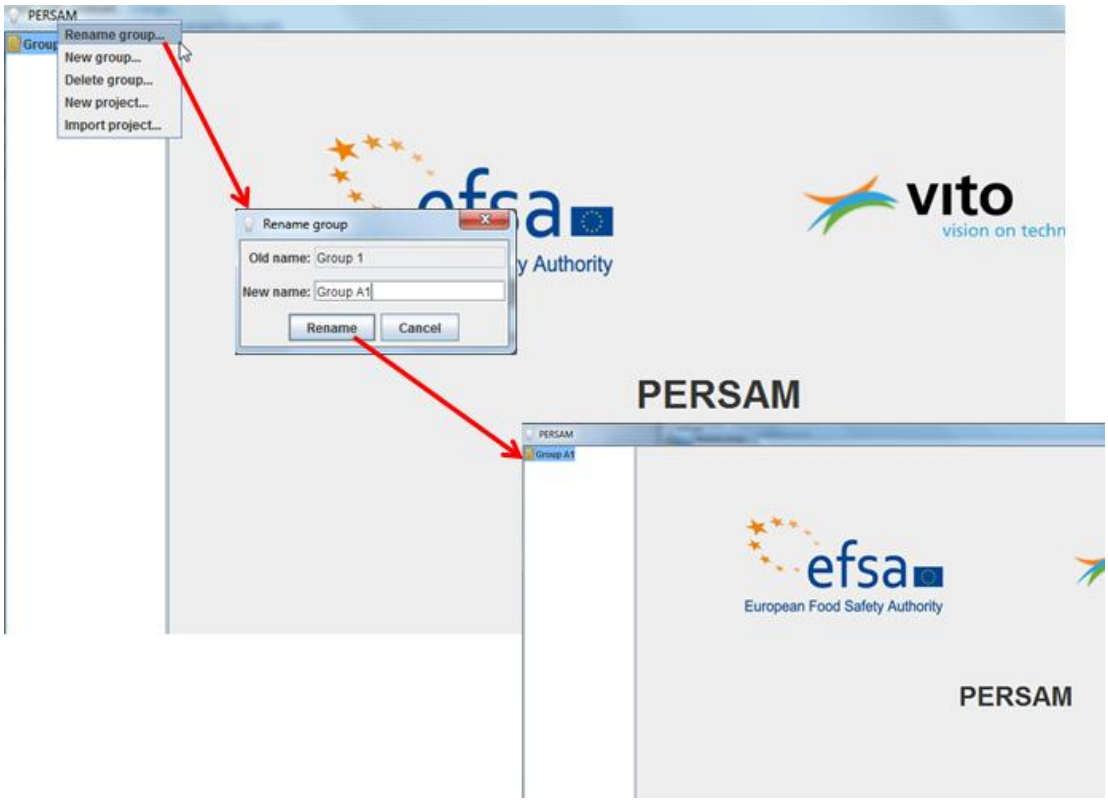



**Figure 20: Rename group**

### 4.1.3. Delete group

The user can delete an existing group in the tree structure.

1. Select a group
2. Right mouse click and select 'Delete group', while you keep the cursor on the selected group.
3. Following message appears: *Delete the following group and all its contents?*

   → Yes: delete the selected group

   → No: don't delete the selected group

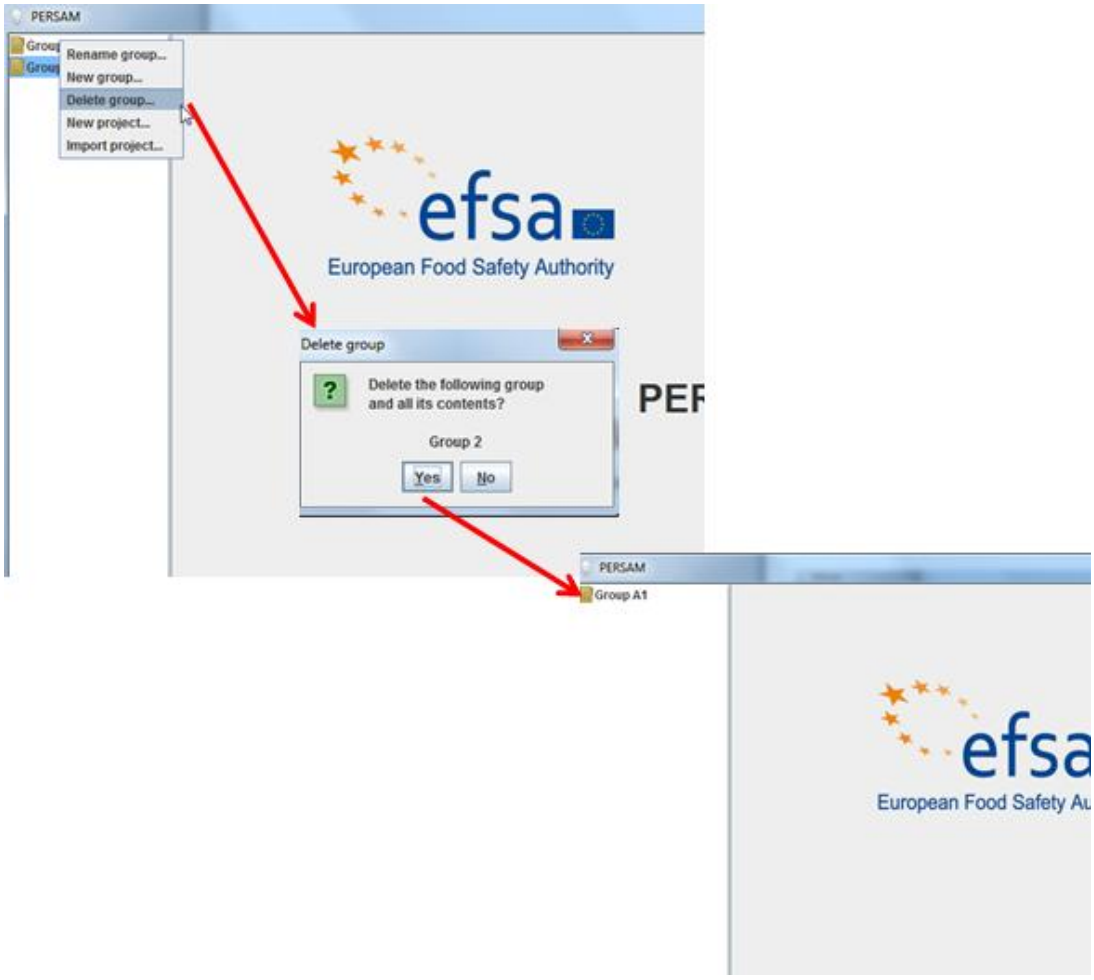



**Figure 21: Project management - Delete a group**

## 4.2. Project

Projects can be organized freely by the user in a tree structure similar to a file system: directories (called 'group' in the tool) which can contain other directories and files (the projects in the tool)
When clicking on a project in the project tree manager at the left side of the screen, the project main screen appears. In this screen, the user can modify the project's name, its description, and the documents attached to the project. At the bottom right of the screen, there are 2 buttons that are disabled if no changes have been made. As soon as a change has been made, the buttons become active. Clicking the undo button will revert all changes made. Clicking the save button will persist the changes.
In the project tree, a fixed set of sub-items of the project are shown: fixed parameters, settings, substances, TIER-1, TIER-2B, TIER-2C, and TIER-3.

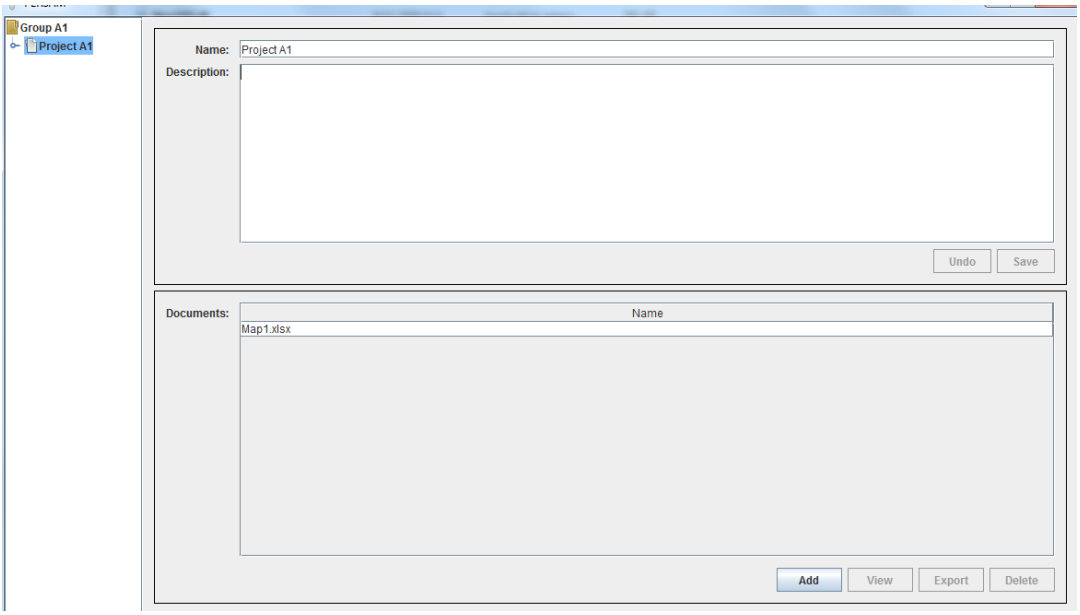



**Figure 22: Project main screen**

**Documents**
The user can add relevant documents to the project.
Other document related functionalities are view, export and delete a document.

**Related project functionalities**:

- New project
- Rename project
- Copy/Paste project
- Delete project
- Import project

- Export project

### 4.2.1. New project

The user creates a new project.

1. If you want to create new project in a group, select first the group and right mouse click, otherwise right mouse click in the left pane of the startup window.
2. Select 'New project'
3. Give a project name
4. Click on 'Create'

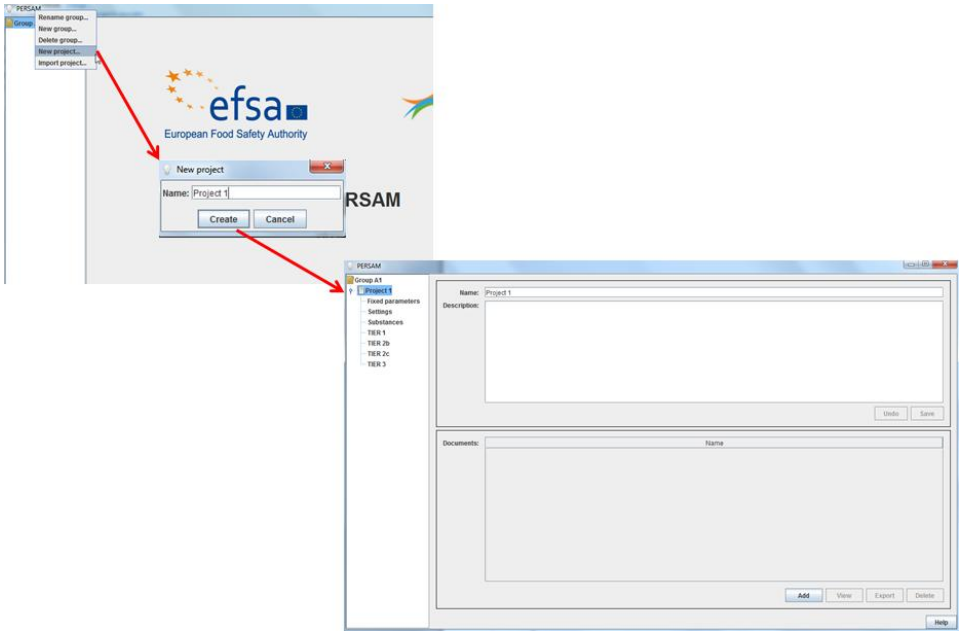



**Figure 23: New project**

### 4.2.2. Rename project

The user changes the project name of an existing project.

1. Select an existing project
2. Go to the project window
3. Change the project name
4. Click on 'Save'

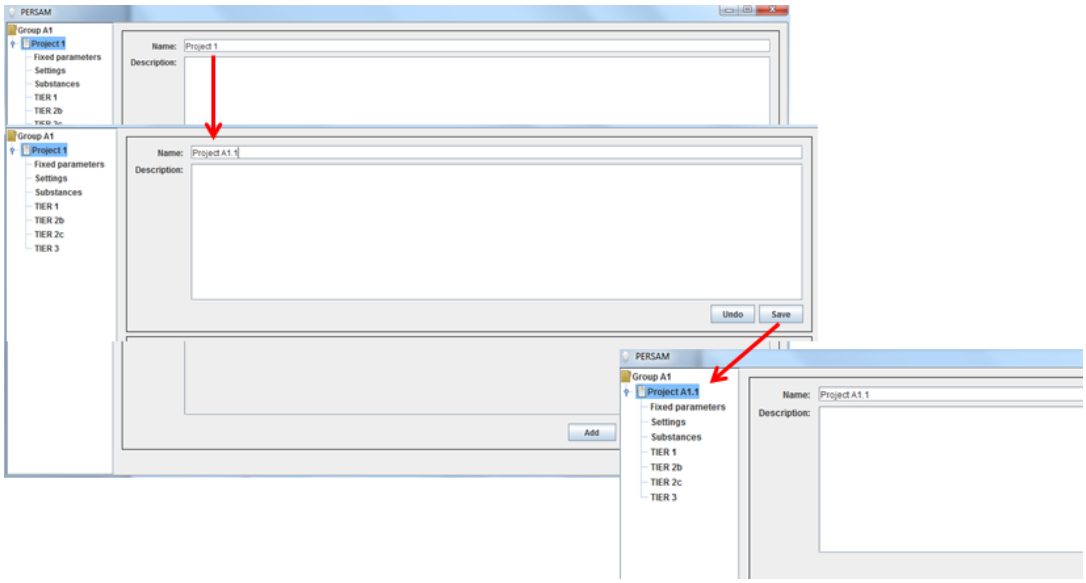



**Figure 24: Rename project**

### 4.2.3. Copy/Paste project

The user exports a project to clipboard (copy).

1. Select an existing project
2. Right click and select 'Copy project'
   The application makes a copy of the project to clipboard.

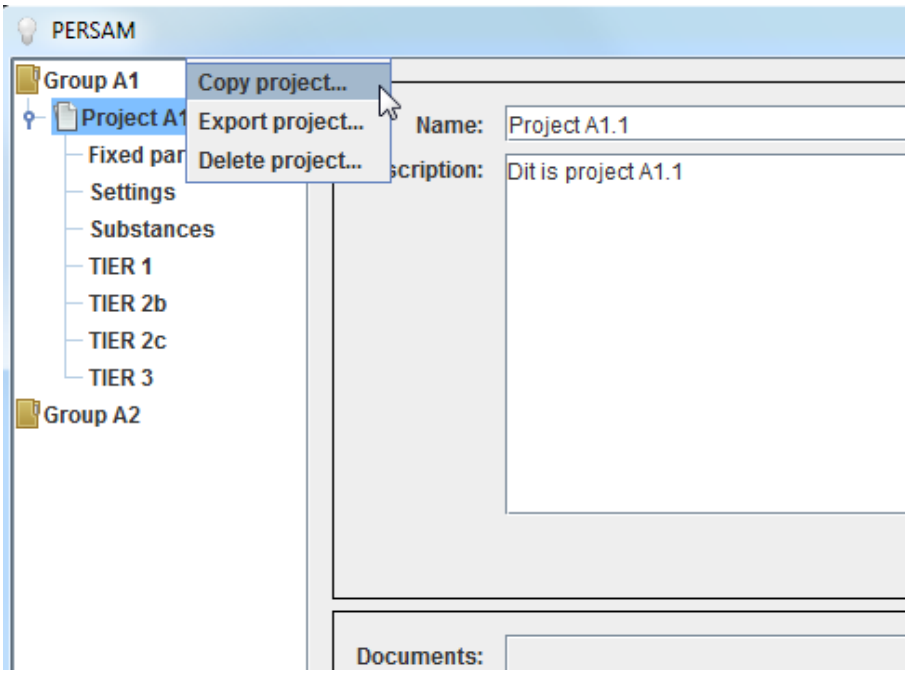



**Figure 25: Project management - Copy project**

3. Select the group where you want to place the copied project
4. Right click and select 'Paste project'

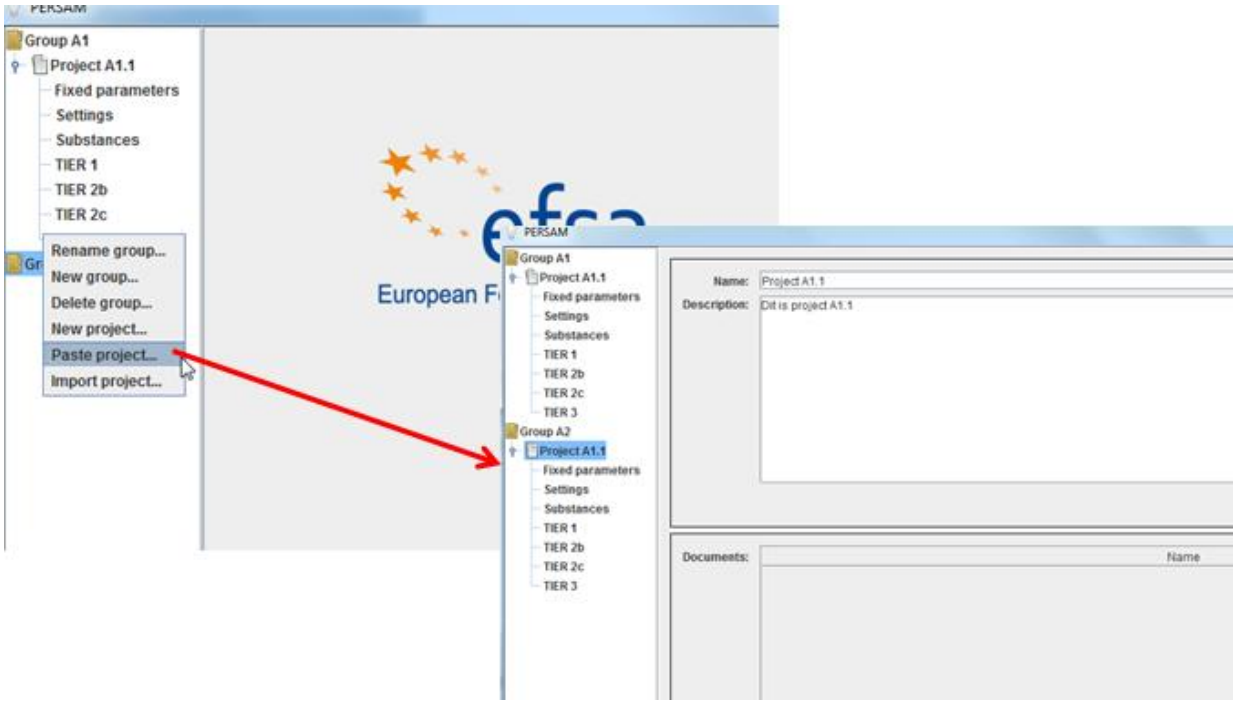



**Figure 26: Project management - Paste project**

5. Rename the project

### 4.2.4. Delete project

The user can delete an existing project.

1. Select a project
2. Right mouse click and select 'Delete project', while you keep the cursor on the selected project.
3. Following message appears: *Delete the following project?*

   → Yes: delete the selected project

   → No: don't delete the selected project

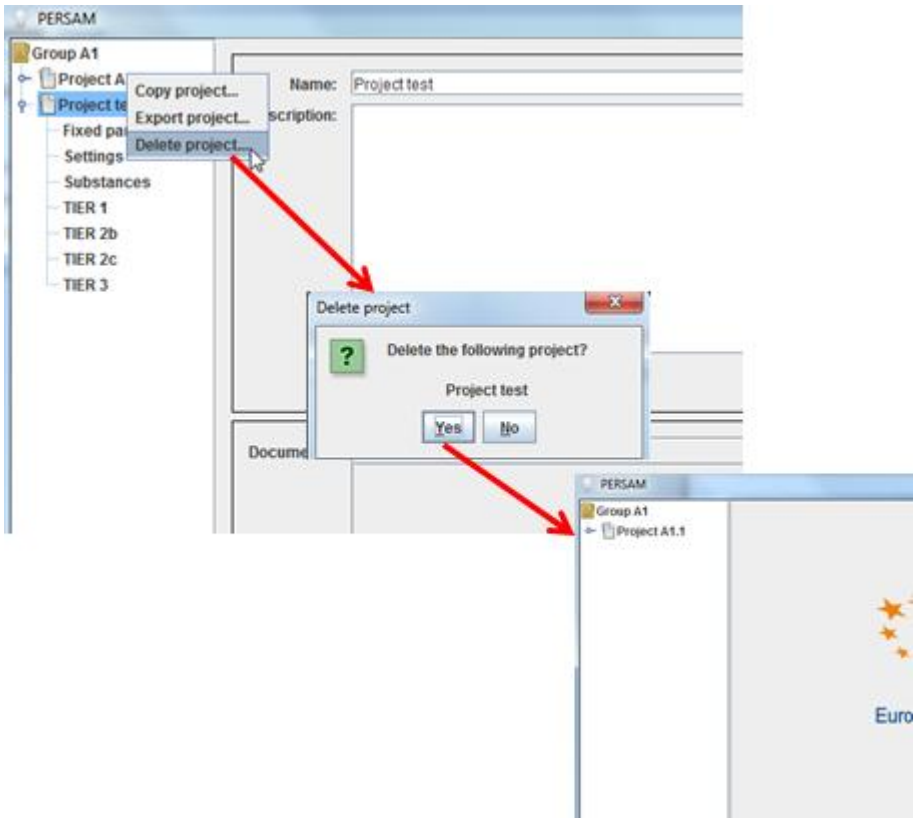



**Figure 27: Project management - Delete project**

### 4.2.5. Import project

The user defines new project from a previously exported project.
This functionality can also be used when you install a new version of PERSAM. Before the installation export the projects and after the installation import the projects.

1. Select the group where you want to import a project
2. Right mouse click and select 'Import project', while you keep the cursor on the selected group
3. There appears a popup window where you select the export file .
4. Click on 'Open' and the project is imported into the application.

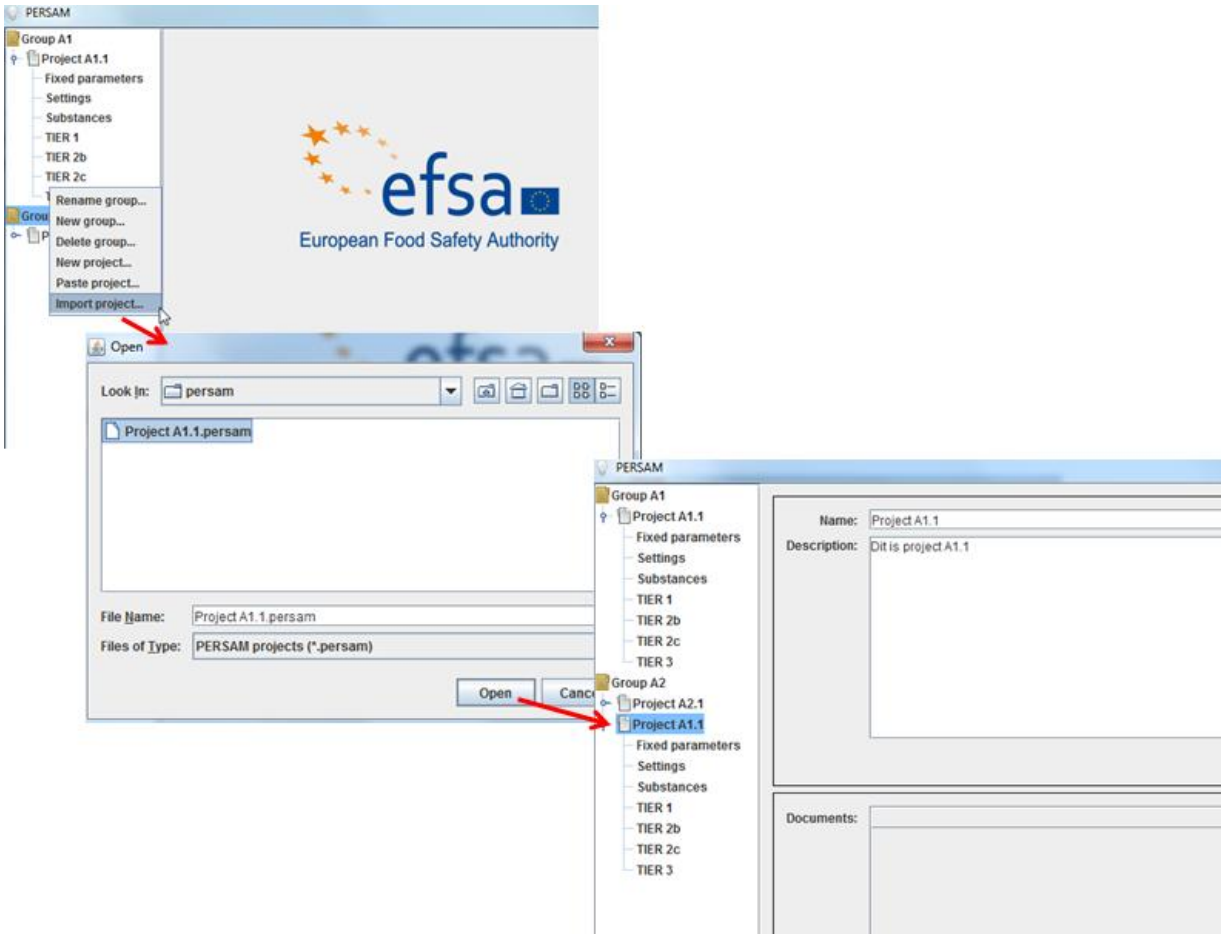



**Figure 28: Project management - Import project**

### 4.2.6. Export project

The user exports a project to a file. This functionality can also be used when you install a new version of PERSAM. Before the installation export the projects and after the installation import the projects.

1. Select a project
2. Right mouse click and select 'Export project', while you keep the cursor on the selected project.
3. There appears a popup window where you define the name of the export file .
4. Click on 'Save' and the project is exported to the export file.

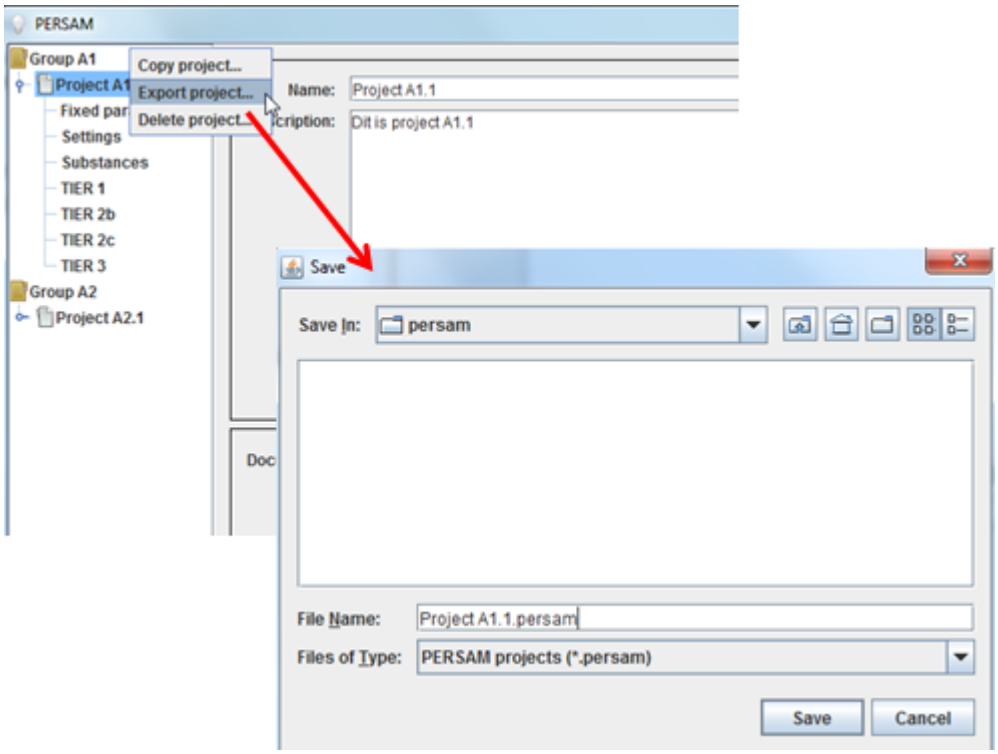



**Figure 29: Project management - Export project**

### 4.2.7. Document management

The user can add relevant documents to the project.
Other document related functionalities are view, export and delete a document.

Next document types are supported:

- Excel
- Word
- PDF
- TXT
- CSV

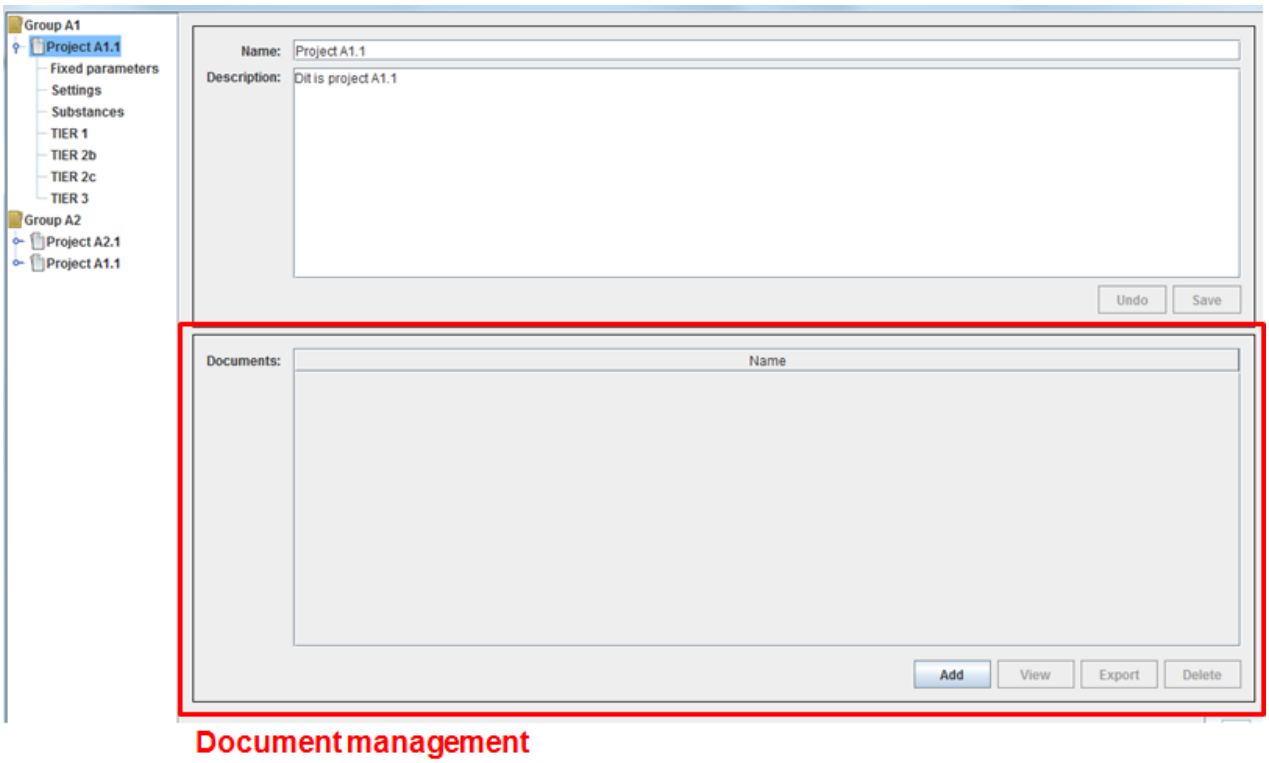



**Figure 30: Project - Document management**

#### 4.2.7.1. Add document

The user can add a relevant document to the project.

1. Click on 'Add'
2. There appears a popup window where you select a particular document .
3. Click on 'Open' and the document is added to the project.

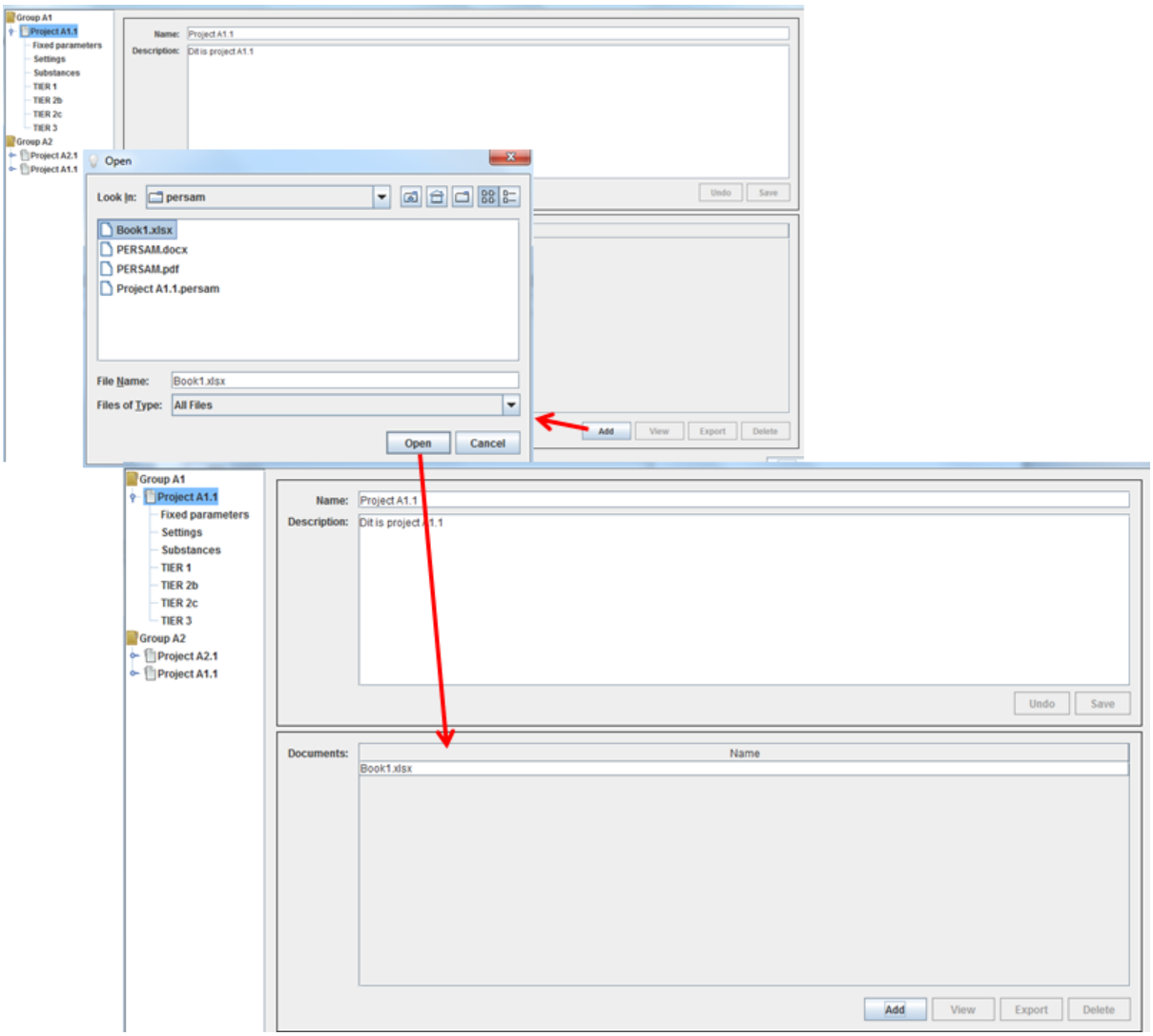



**Figure 31: Document management - Add document**

#### 4.2.7.2. View document

The user can view the documents related to the project.

1. Select a particular document
2. Click on 'View' and the document will be opened.
   The user can only consult excel files, word documents, pdf documents, txt files and csv files.

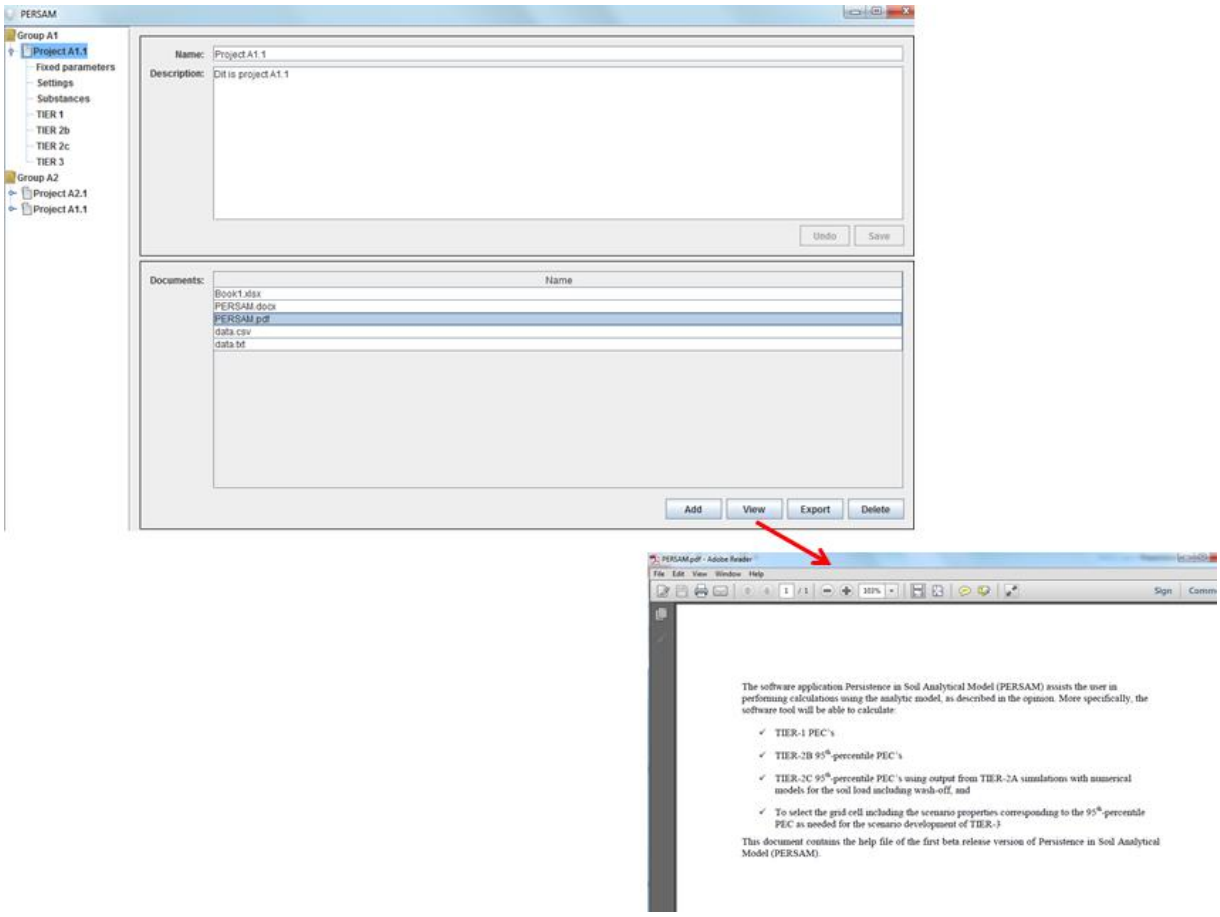



**Figure 32: Document management - View document**

#### 4.2.7.3. Export document

The user can export documents related to the project.

1. Select a particular document
2. Click on 'Export'
3. There appears a popup window where where you define the export name and the location for the export file .
4. Click on 'Save'

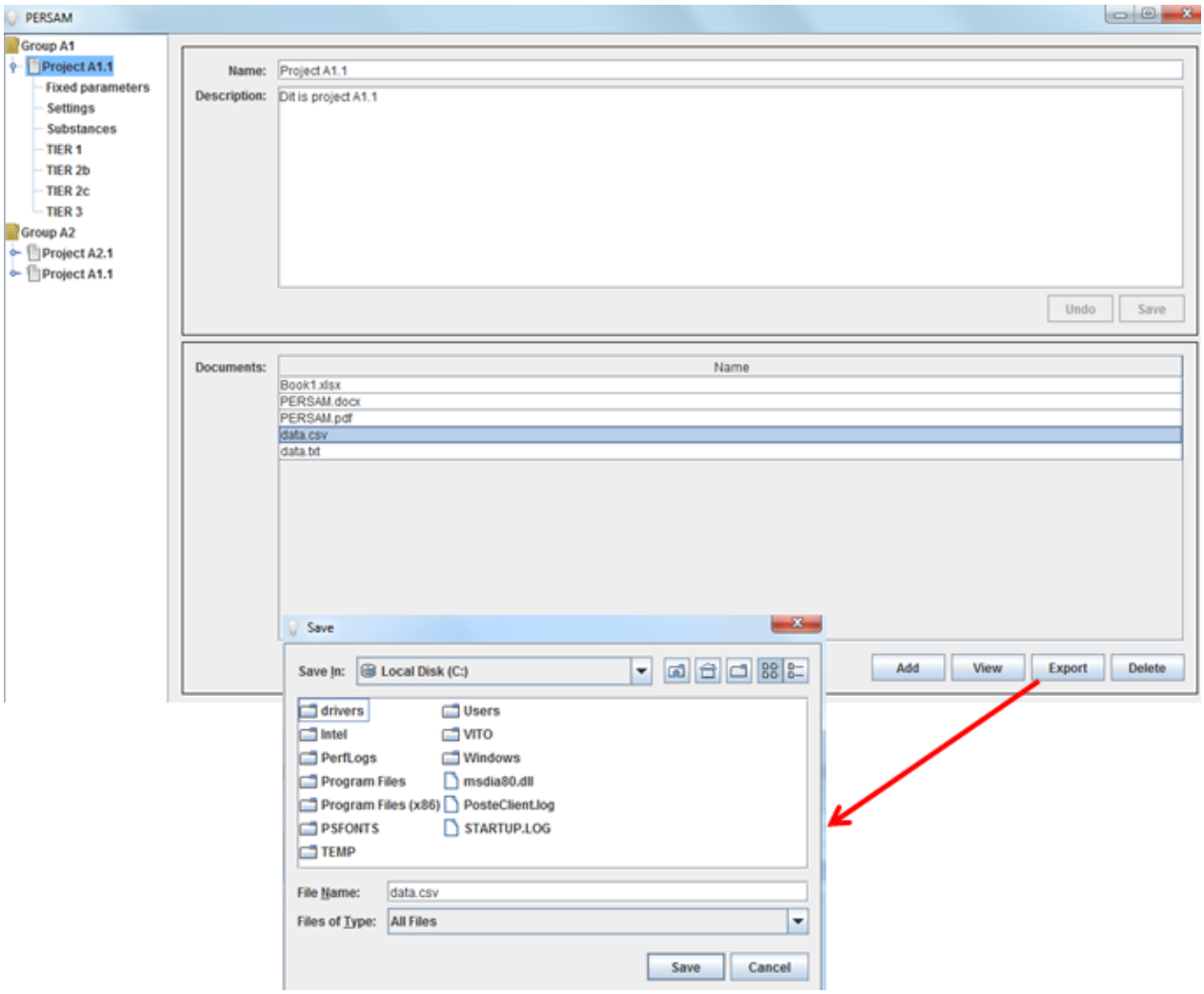



**Figure 33: Document management - Export document**

#### 4.2.7.4. Delete document

The user can delete a document related to the project.

1. Select a particular document
2. Click on 'Delete'
3. Following message appears: *Are you sure you want to delete document "[document name]"?*
   → Yes: delete the selected document

   → No: don't delete the selected document

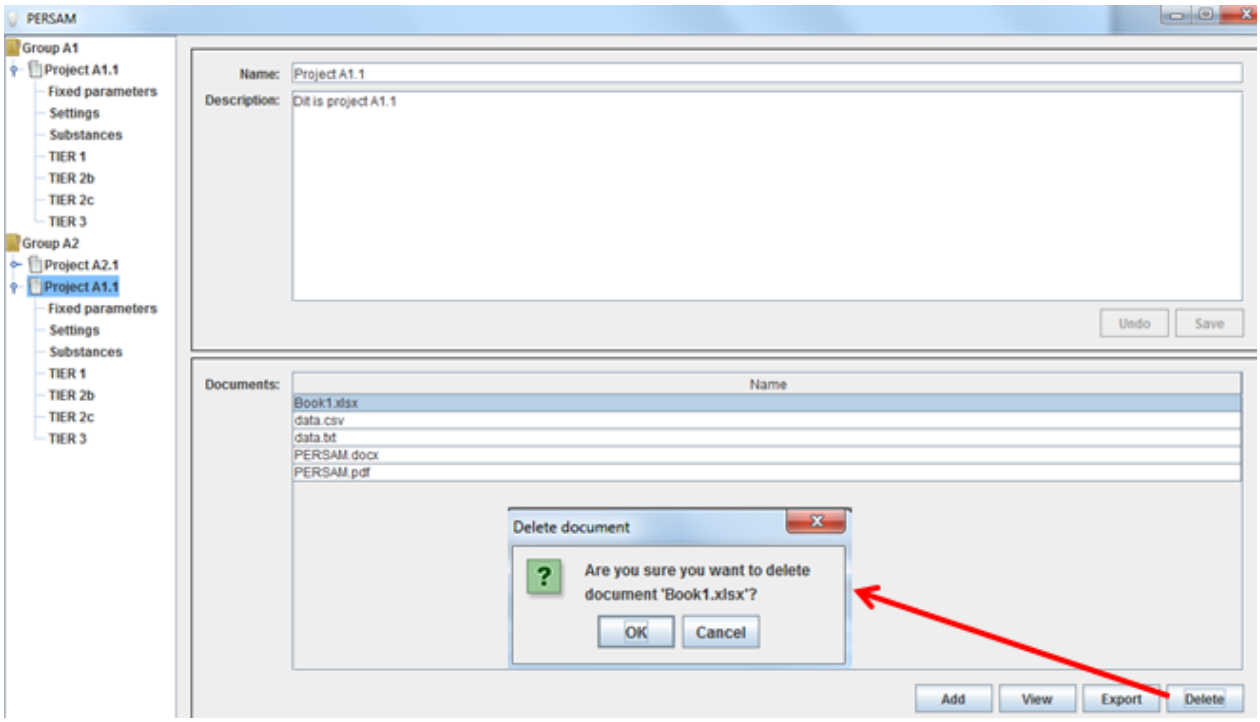



**Figure 34: Document management - Delete document**

## 5. Fixed parameters

The fixed parameters section gives an overview of all parameters that are used in the calculations but cannot be changed by the user.

**Table 1:** Fixed parameters

| | Symbol | Unit | Default values |
|---|---|---|---|
| **Parameter** | | | |
| Ecotoxicological averaging depth | $z_{eco}$ | cm | 1; 2.5; 5; 20 |
| Plough depth | $z_{til}$ | cm | 20 |
| Gas constant | R | $kJ.mol^{-1}.K^{-1}$ | 0.008314 |
| Reference temperature | $T_{ref}$ | K | 293.15 |
| Time period since application over which concentrations are averaged | $t_{avg}$ | days | 0; 7; 14; 21; 28; 56 |

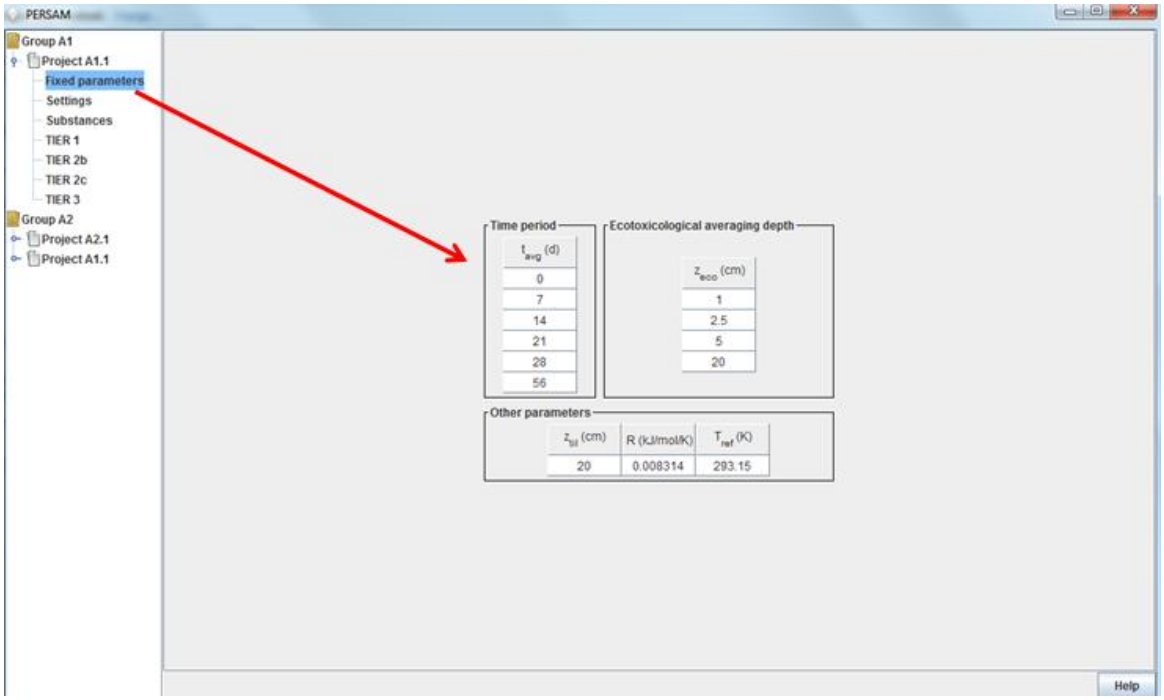



**Figure 35: Fixed parameters**

## 6. Settings

In the settings section, the user can configure the calculations.

- The calculation can be done for several zones. At least 1 zone must be selected.
- Several endpoints can be calculated. At least 1 endpoint must be selected.
- The CAPRI crop for which the calculations must be done.
- For TIER 2c, the user must enter the fraction that reached the soil ($F_{soil, max}$) to use here. This parameter is not used in the other TIERs.

The undo and save buttons are disabled as long as the user did not change settings in this screen. As soon as changes have been made, the undo button becomes enabled. As soon as the changes represent a valid configuration (at least 1 zone selected, etc.) the save button becomes available as well.

Following table gives an overview of the selection parameters.

**Table 2:** Selection parameters

| | | Description | TIERS |
|---|---|---|---|
| **Parameter** | | | |
| Zone | North<br>Center<br>South | By default all zones are checked | TIER-1, TIER-2B, TIER-2C and TIER-3 |
| Endpoints | Concentration in total soil $C_T$<br><br>Concentration in liquid phase $C_L$ | | TIER-1, TIER-2B, TIER-2C and TIER-3 |
| CAPRI Crop | | see CAPRI crop list | TIER-1, TIER-2B, TIER-2C and TIER-3 |
| Fraction that reaches the soil $F_{soil, max}$ | | | TIER-2C |
| Additional exports | Exported generated maps as ESRI ASCII files | By default this parameter is not selected | TIER-1, TIER-2B, TIER-2C and TIER-3 |

When the checkbox in the 'Additional exports' section is enabled, the tool will export all generated maps in TIERs 2b, 2c, and 3 to a given location on the file system in ESRI ASCII grid file format. Note that this will require a significant amount of disk space. Existing files will be overwritten. The target folder can be selected by clicking the 'Select folder' button: a chooser dialog pops up.

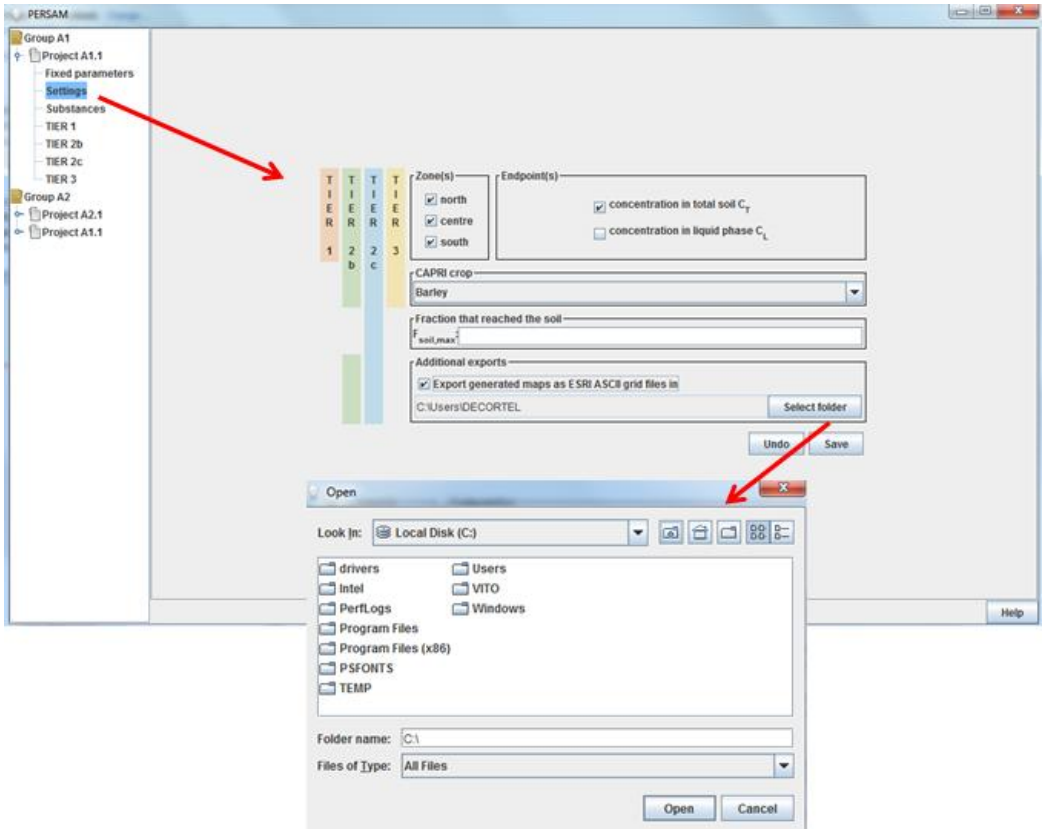



**Figure 36: Settings section**

If changes have been made, and the user navigates away from the screen without clicking the save button, the following warning pops up.

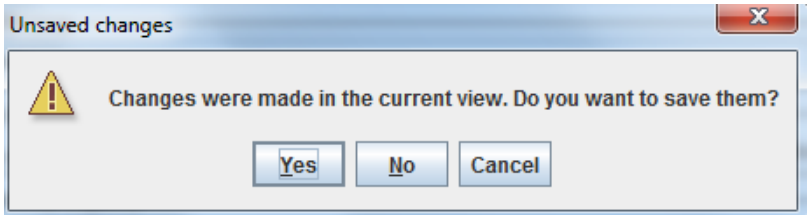



**Figure 37: Dialog Unsafed changes**

- Clicking the yes button has the same effect as clicking the save button and navigating away from the screen.
- Clicking the no button has the same effect as clicking the undo button and navigating away from the screen.

- Clicking the cancel button returns to the settings screen as if nothing happened.

If the user returns to this section after some or all of the TIER calculations have been done, and he changes settings, these changes will introduce discrepancies between the project configuration and the already calculated results. Therefore all results will be deleted prior to persisting these configuration changes.

## 7. Substances

Substances are organized in a tree structure. The root of this tree contains the parent substance, for which the annual application rate (kg/ha), as well as the time between applications must be entered by the user. The tool allows the definition of up to 2 levels of metabolites: substances that are formed out of substances in the level above them. Each level can contain up to 4 metabolites.

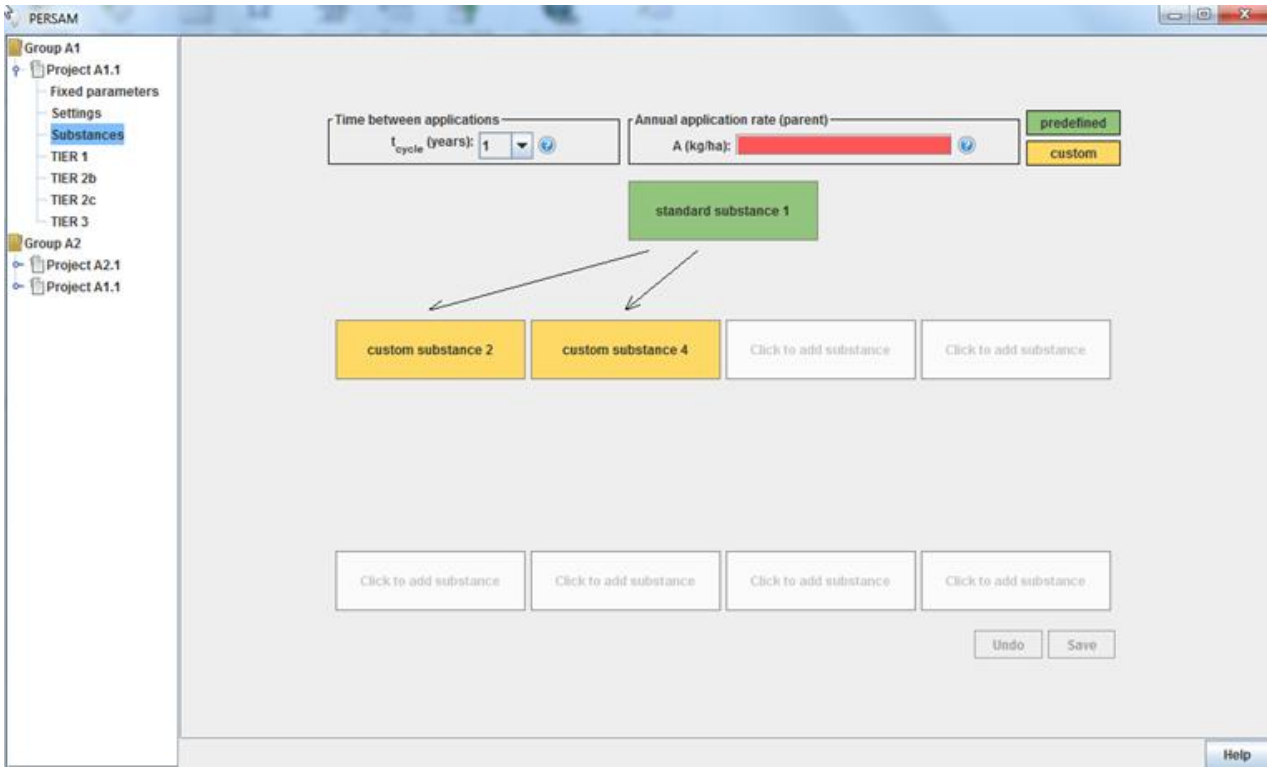



**Figure 38: Substances section**

A substance (parent or metabolite) is configured by clicking on a place holder in the tree. The tool contains a number of predefined substances with a fixed configuration. Apart from these, the user can also define custom substances. The color of the place holders indicates which of those 2 types of substances is used. Arrows between the place holders can be configured by clicking on them. Only the arrows between place holders that contain a substance can be configured.

Next table gives an overview of the substance-specific parameters.

**Table 3:** Substance-specific parameters

| | Symbol | Unit | Default value |
|---|---|---|---|
| **Parameter** | | | |
| Half life for degradation of the substance | DegT50 | days | |
| Organic matter/water distribution coefficient | $K_{om}$ | l/kg | |
| Organic carbon/water distribution coefficient | $K_{oc}$ | l/kg | |
| Molar mass | M | $g.mol^{-1}$ | |
| Arrhenius activation energy | E | $kJ.mol^{-1}$ | 65.4 |
| Formation fraction metabolite | $F_f$ | | |
| Annual application rate | A | kg/ha | |

**Related functionalities**:

- Configure a predefined substance (parent or metabolite)
- Configure a custom substance (parent or metabolite)
- Delete a substance (parent or metabolite)
- Configure a link between substances (parent, metabolites)
- Delete a link between substances (parent, metabolites)

### 7.1. Configure predefined substance

The user defines a predefined substance (parent or metabolite)

1. Click on a place holder in the tree and the screen 'Configure substance' appears.
2. Select one of the build in substances in the drop down list
3. The screen shows automatically the related parameters of the selected substance. These parameters are not editable.

4. Click 'OK'

Note: If the user selects the code, the substance related parameters become editable and the user can configure a customized substance.

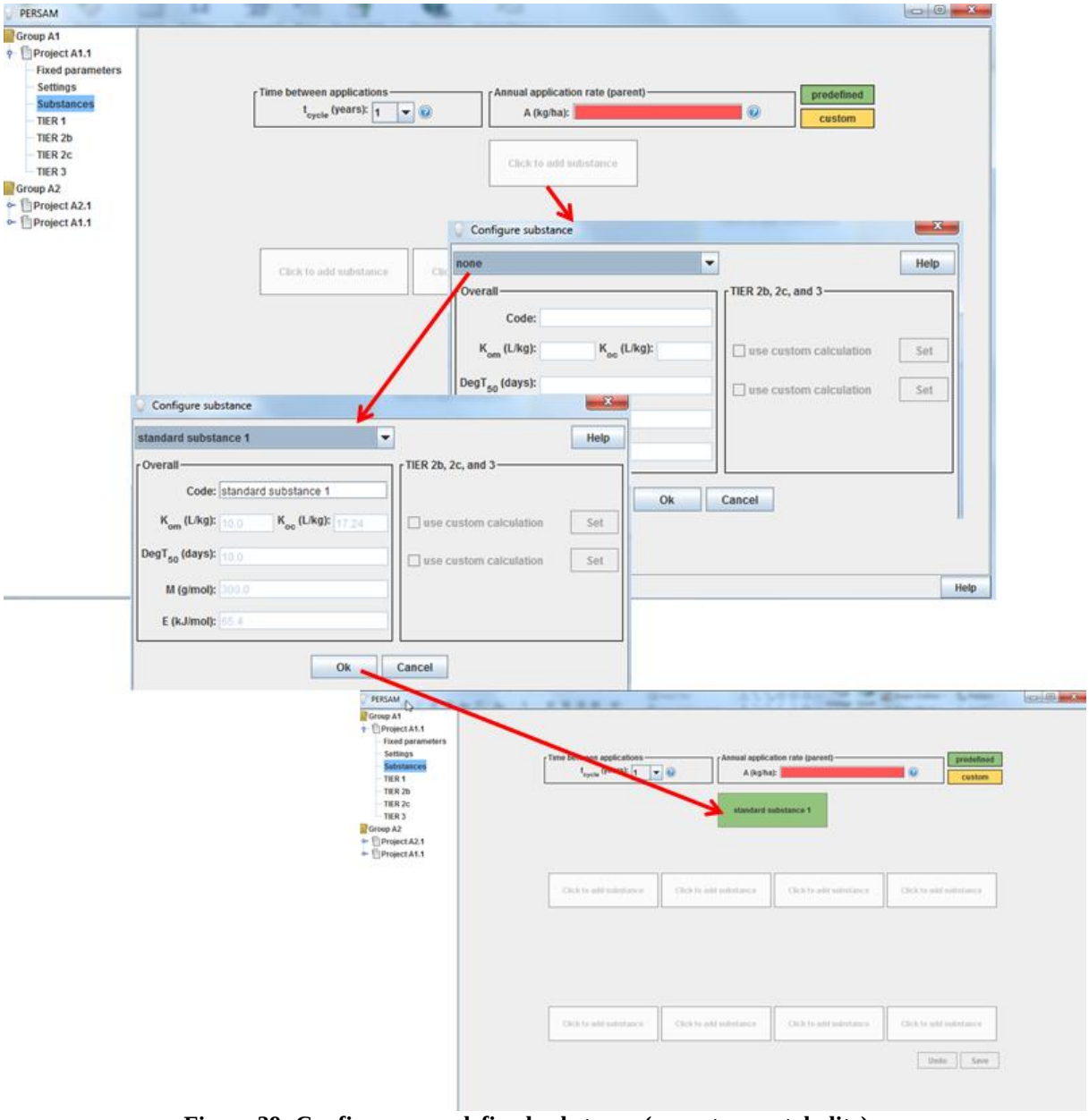



**Figure 39: Configure a predefined substance (parent or metabolite)**

## 7.2. Configure custom substance

The user defines a customized substance (parent or metabolite) starting from a defined substance or defining a new substance.

**Starting from a defined substance:**

1. Click on a place holder in the tree and the screen 'Configure substance' appears.
2. Select one of the build in substances in the drop down list
3. The screen shows automatically the related parameters of the selected substance, not editable.
4. Select then 'custom' in the list or put your cursor in the code field that identifies the substance
5. Define a new code and change the substance related parameters
6. Click on 'OK'

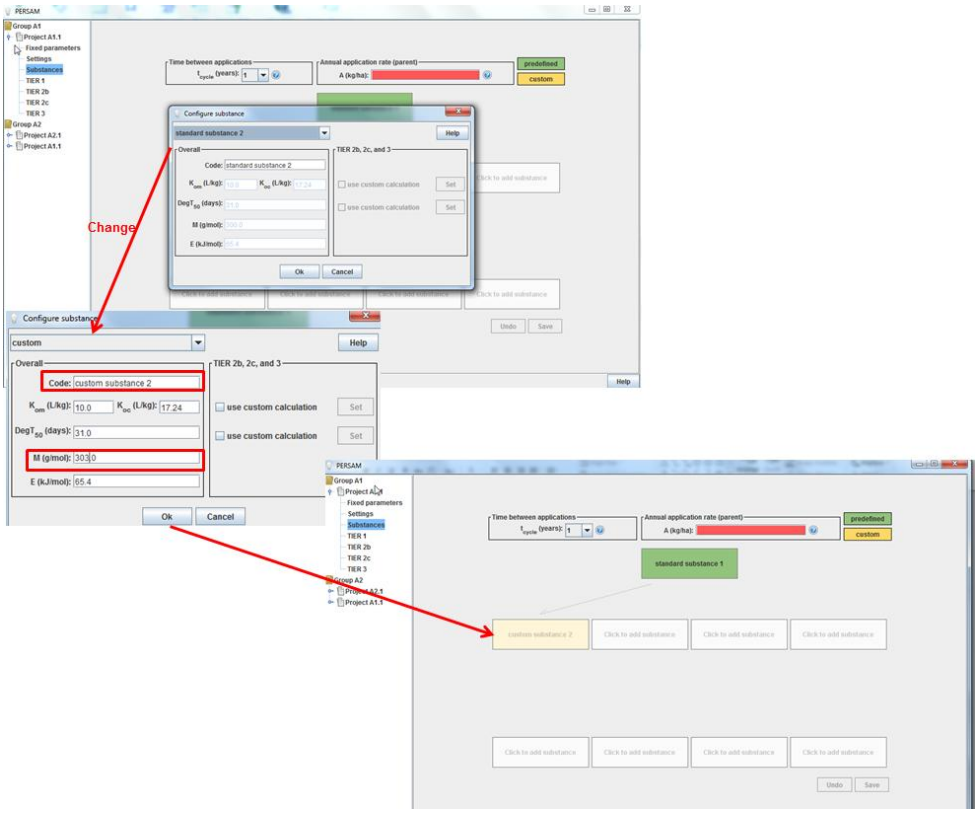



**Figure 40: Configure a customized substance, starting from a predefined substance**

**Defining a new customized substance:**

1. Click on a place holder in the tree and the screen 'Configure substance' appears.
2. Select the value 'Custom' in the drop down list
3. Define the code and the substance related parameters. The 'OK' button becomes active when all parameters are filled in.

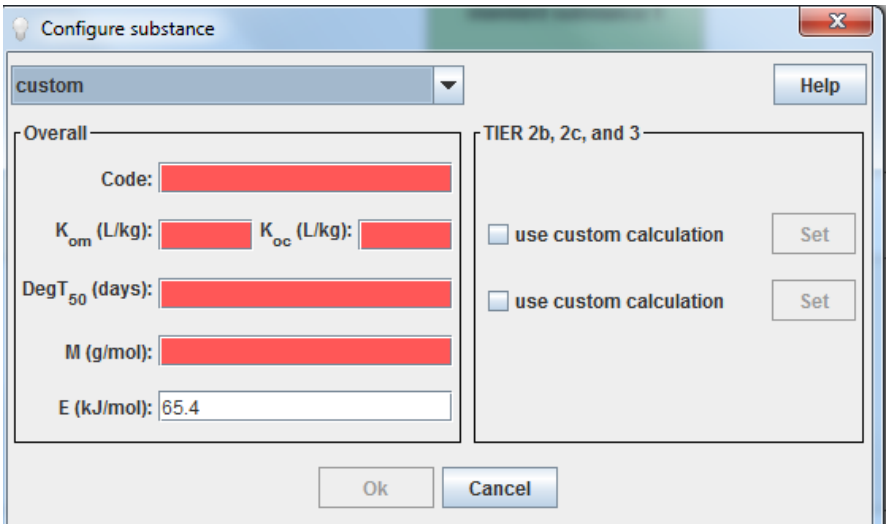



**Figure 41: Configure a new customized substance**

4. Click on 'OK'

## 7.3. Configure custom calculations

The user has the possibility to define relationships between Kom, DegT50 and soil properties.

**Configure a custom calculation for Kom or for DegT50**

1. Click on a place holder in the tree and the screen 'Configure substance' appears.
2. Configure a predefined substance (see Configure predefined substance ) or a custom substance (see Configure custom substance )
3. Select the checkbox 'Use custom calculation' for Kom or for DegT50
4. Click on the related set button and the window 'Define custom calculation' appears

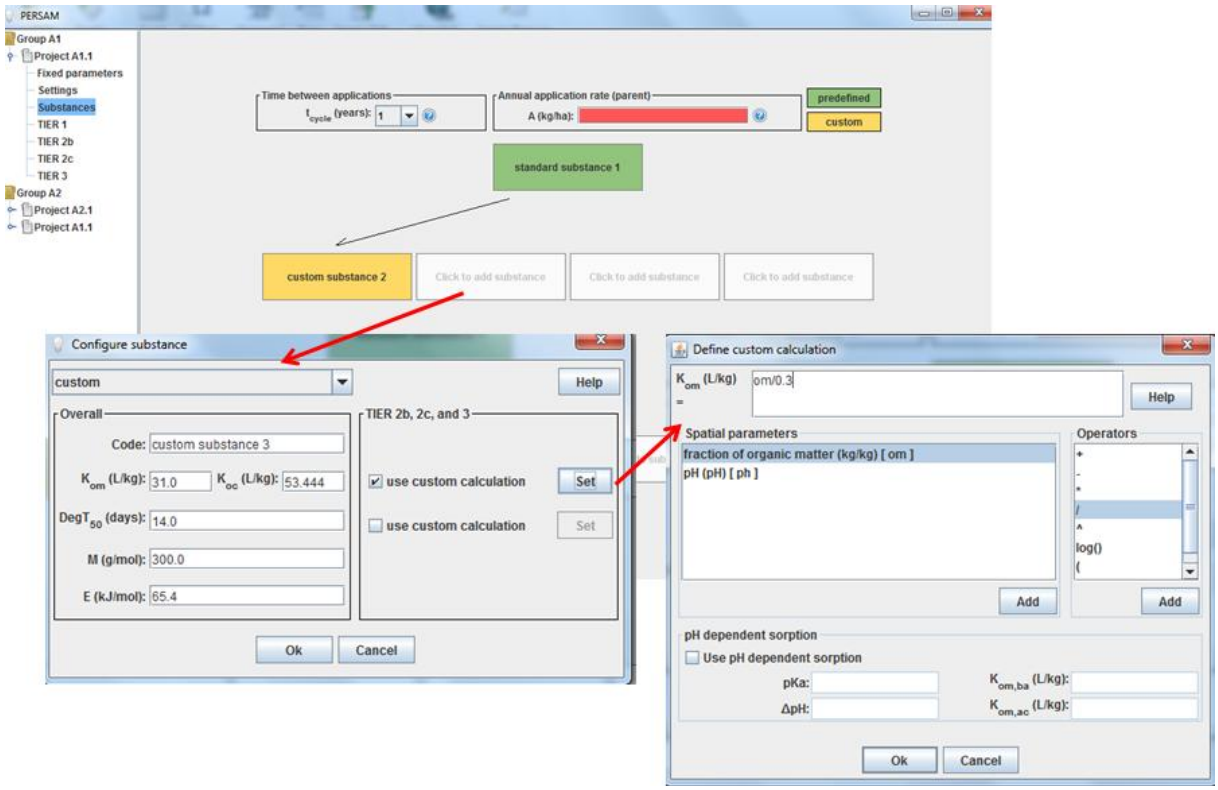



**Figure 42: Define custom calculation for Kom**

***Calculation based on spatial parameters:***

1. Select a spatial parameter and click on add
2. Select an operator and click on add
3. Select another parameter or enter a value in the formula rectangle.
4. Click 'OK'

***Calculation based on pH dependent sorption:***

1. Select the checkbox 'Use pH dependent sorption'
2. Enter the parameters related to pH dependent sorption
3. Click 'OK'.

$$K_F = m_{om} \frac{K_{om,ac} + K_{om,ba} \frac{M_{ba}}{M_{ac}} 10^{pH - pK_a - \Delta pH}}{1 + \frac{M_{ba}}{M_{ac}} 10^{pH - pK_a - \Delta pH}}$$

pKa: negative logarithm of the dissociation constant
ΔpH: pH correction factor
$K_{OM, ba}$: organic matter/water distribution coefficient under basic conditions
$K_{OM, ac}$: organic matter/water distribution coefficient under acid conditions

*Formula for pH dependent sorption*

Following spatial parameters and operators are provided in the 'Define custom calculation' window:

**Table 4:** Spatial parameters available in the 'Define custom calculation' window

| | **Code** |
|---|---|
| **Spatial parameter** | |
| Fraction of organic matter (kg/kg) | [om] |
| pH (pH) | [ph] |

Operators available in the 'Define custom calculation' window are:

| | | | | | |
|---|---|---|---|---|---|
| + | - | * | / | % | ^ |
| ( ) | Sin( ) | Cos( ) | Tan( ) | Asin( ) | Acos( ) |
| Atan( ) | Sinh( ) | Cosh( ) | Tanh( ) | Asinh( ) | Acosh( ) |
| Atanh( ) | Ln( ) | Log( ) | Abs( ) | Rand( ) | Sqrt( ) |
| Erf( ) | Erfc( ) | Gamma( ) | Exp( ) | Cot( ) | Log2( ) |

### 7.4. Delete a substance

The user can remove a configured substance in the tree structure.

1. Click on a configured substance in the tree structure.
2. Select the value 'None' in the drop down list

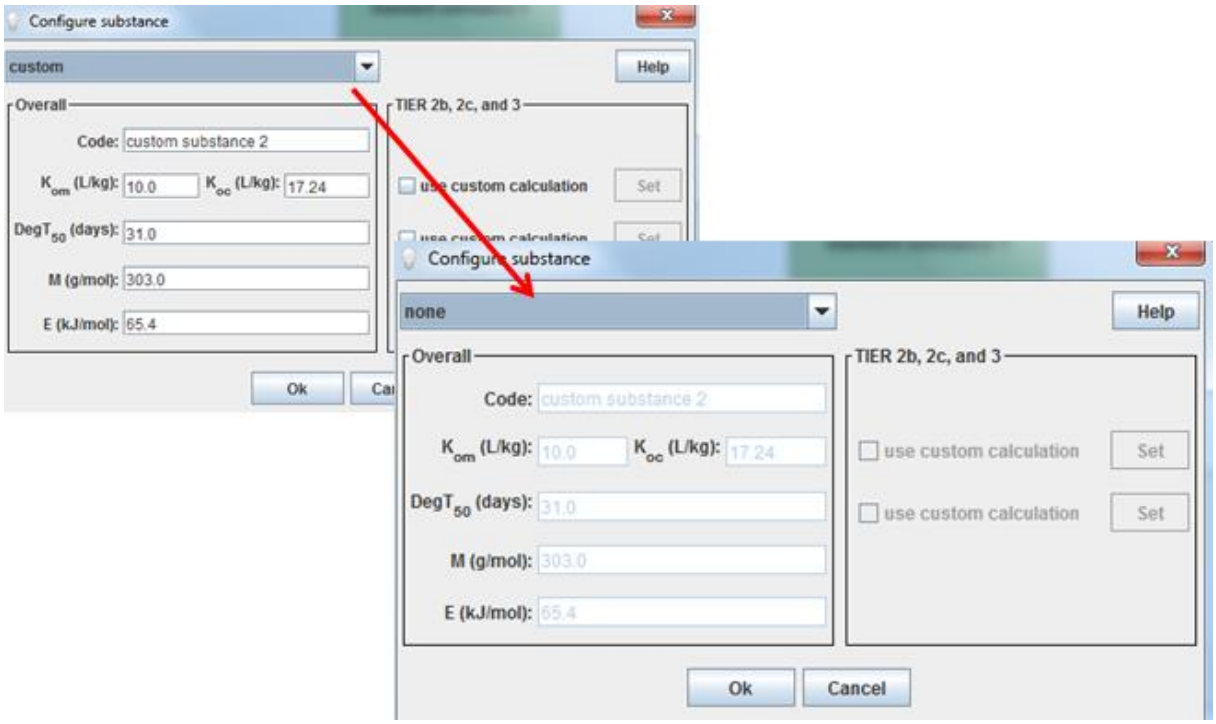



**Figure 43: Delete a configured substance**

3. Click 'OK' and the substance is removed from the tree structure.

## 7.5. Configure link

Links are represented as arrows between the place holders in the tree structure.

1. Click on an arrow between two place holders that contain a substance and the dialog 'Configure link' appears
   The source and target substance fields are informative: they cannot be changed.
2. Enable the checkbox 'Link enabled'.
   Unchecking the' link enabled' checkbox will disable an arrow (grey), keeping it enabled will enable the arrow (black).
3. Define the formation factor
4. Click 'OK'

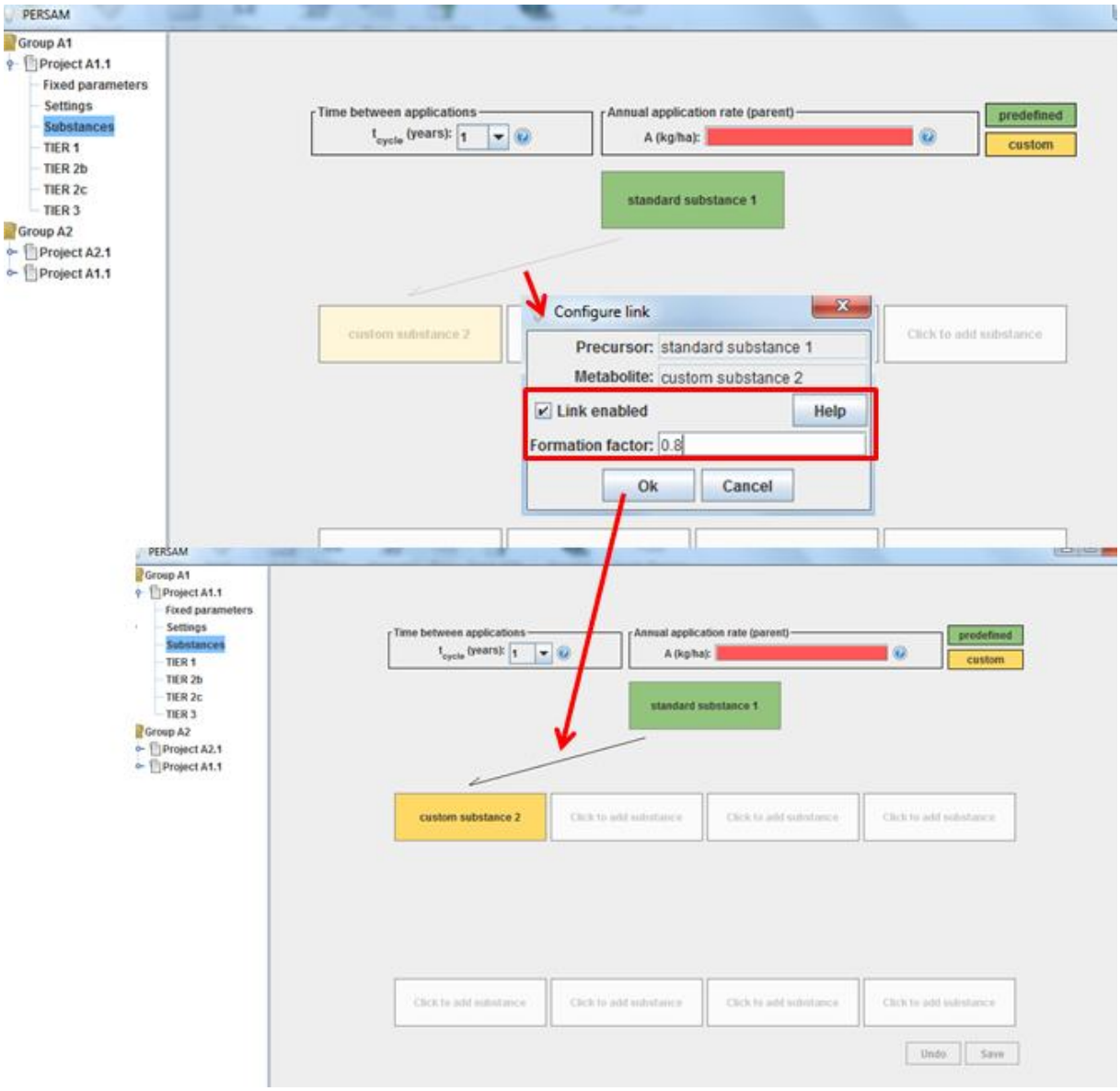



**Figure 44: Configure a link**

If a substance is configured where no arrows point to, this substance is removed when the user clicks the save button. This will also disable all arrows that start in that removed substance. If this renders additional substances into orphans (no arrows arrive there), then these substances are removed as well.

### 7.6. Delete a link

The user can remove a configured link between two place holders in the tree structure.

1. Click on a configured link in the tree structure.
2. Uncheck the' link enabled' checkbox and the arrow (grey) will be disabled.

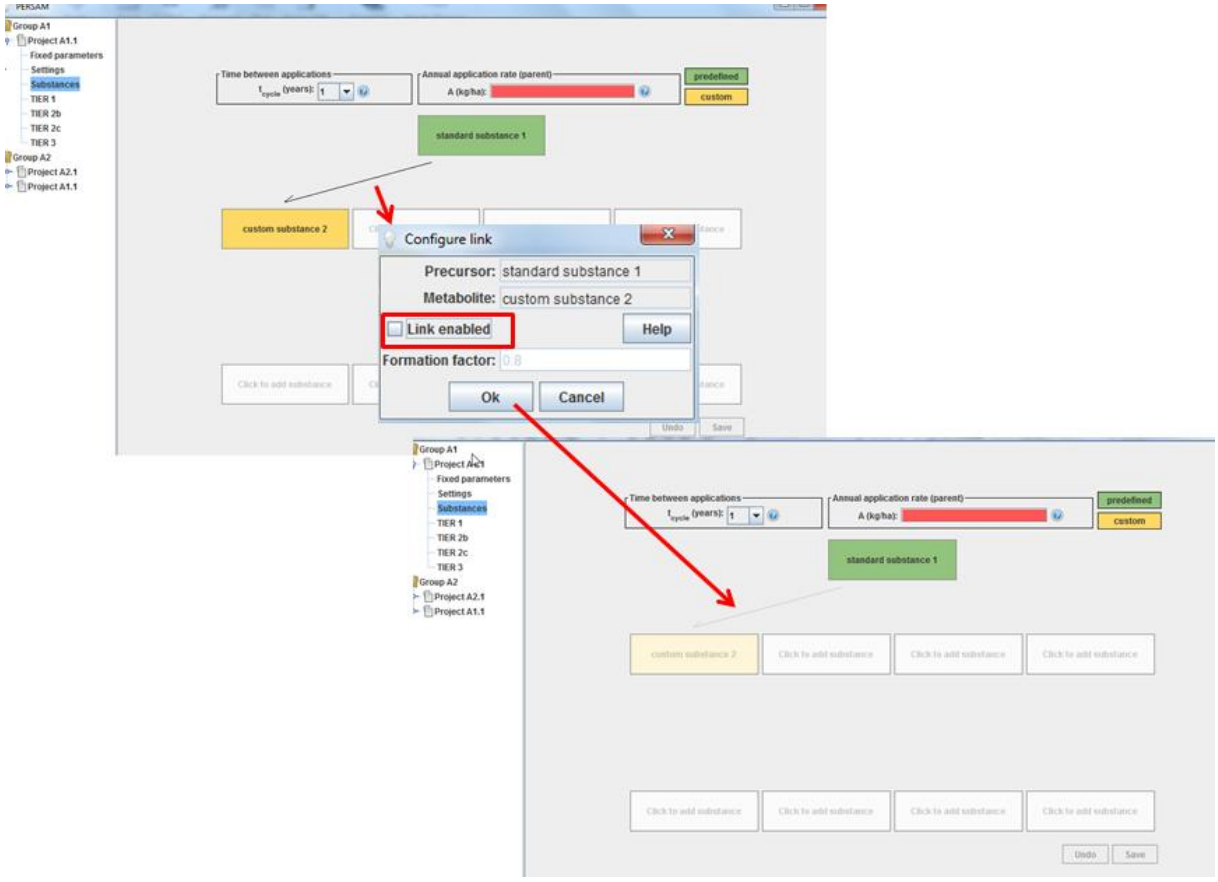



**Figure 45: Delete a link**

## 8. TIER-1

TIER-1 consists of calculations for six scenarios: three regulatory zones North, Center , South and two endpoints in soil, i.e. concentration in pore water and total concentration in soil. The user should select one or more scenarios (North, Center, South) with its associated input parameters, and select one or two endpoints (pore water concentration, total concentration in soil). The application will calculate PEC values for the selected end points and the selected regulatory zones.

The TIER-1 section is shown in following figure.

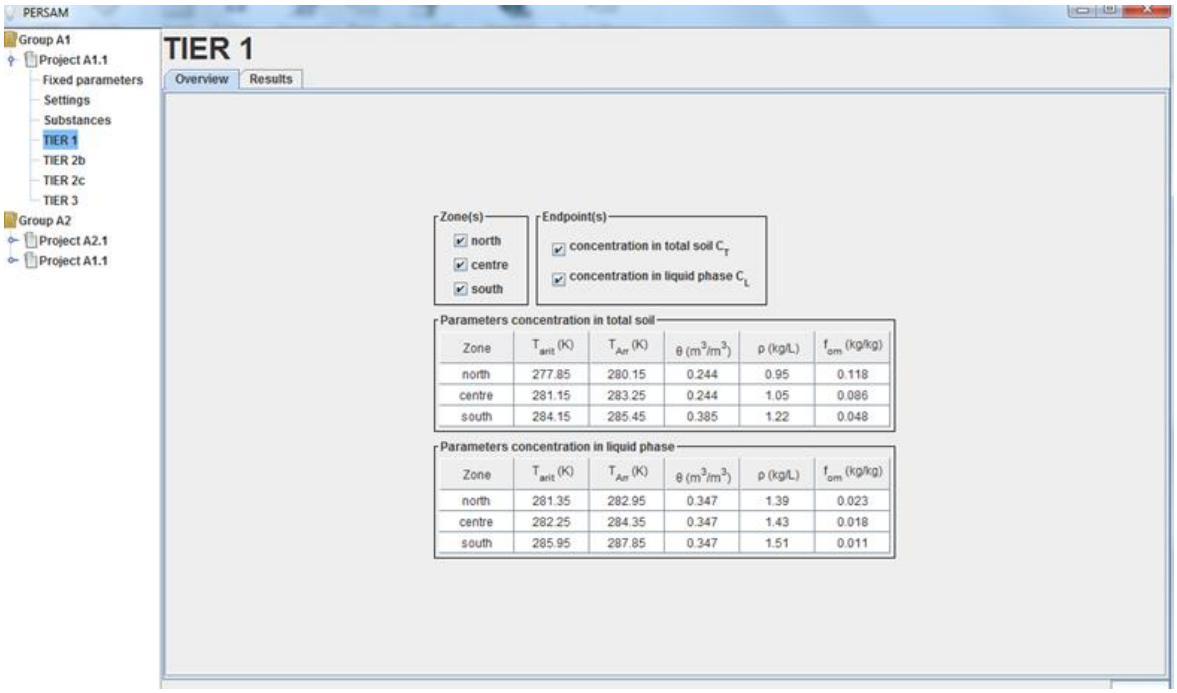



**Figure 46: TIER-1 section**

This screen consists of 2 tabs: overview and results. The overview tab shows the configured settings and the zone and endpoint dependent parameter values that will be used in the calculations.

### 8.1. TIER-1 settings

TIER-1 settings for the calculation of the PEC values are:

- Zone(s) (see settings section)
- Endpoint(s) (see settings section)
- Substances (parent & metabolites) (see substance section)

## 8.2. TIER-1 calculations

The TIER-1 calculations includes the calculation of the PEC values and applying scenario adjustment factor and model adjustment factor

### 8.2.1. Calculations

The calculation of the PEC values will be done in several steps.

Step 1: calculation of the initial concentration in total soil

***Formula 1***

$$C_{T,ini} = \frac{A}{\rho z_{eco}}$$

With:

**Table 5:** Parameters in formula $C_{T,ini}$

| | Symbol | Unit | Default values/Input |
|---|---|---|---|
| **Parameter** | | | |
| Initial total concentration in soil | $C_{T,ini}$ | $mg.kg^{-1}$ | Formule [1] |
| Ecotoxicological averaging depth | $z_{eco}$ | cm | 1; 2.5; 5; 20 cm |
| Annual application rate | A | $kg.ha^{-1}$ | Input field tab Substances |
| Dry bulk density | ρ | $kg.L^{-1}$ | Soil-specific parameter |

Step 2: background concentration in soil just before next application

***Formula 2:***

$$C_{T,plateau} = \frac{z_{eco}}{z_{til}} C_{T,ini} \frac{X}{1-X}$$

***Formula 3:***

$$X = e^{-t_{cycle} f_T k_{ref}}$$

***Formula 4:***

$$T > 0°C \quad f_T = \exp\left(\frac{-E}{R}\left[\frac{1}{T} - \frac{1}{T_{ref}}\right]\right)$$

$$T < 0°C \quad f_T = 0$$

***Formula 5:***

$$k_{ref} = \frac{\ln 2}{DegT_{50}}$$

With:

**Table 6:** Parameters used in step 2

| | Symbol | Unit | Default values/Input |
|---|---|---|---|
| **Parameter** | | | |
| Background concentration in soil just before next application | $C_{T,plateau}$ | $mg.kg^{-1}$ | Formula 2 |
| Ecotoxicological averaging depth | $z_{eco}$ | cm | 1; 2.5; 5; 20 |
| Plough depth | $z_{til}$ | cm | 20 |
| Initial total concentration in soil | $C_{T,ini}$ | mg.kg-1 | Step 1 |
| fraction of the dose left at the moment of the next application | X | | Formula 3 |
| Time between applications | $t_{cycle}$ | days | 365; 730; 1095 |
| Correction factor for temperature | $f_T$ | | Formula 4 |
| degradation rate coefficient at reference temperature | $k_{ref}$ | $days^{-1}$ | Formula 5 |
| Arrhenius activation energy | E | $kJ.mol^{-1}$ | Default 65.4; input field in Substances |
| Gas constant | R | kJ.mol$^{-}$ | 0.008314 |

| | | | |
|---|---|---|---|
| | | $^{1}.K^{-1}$ | |
| Reference temperature | Tref | K | 293.15 |
| Arrhenius weighted average soil temperature | $T_{Arr}$ | K | Corresponding to parameter T in formula 4<br>Soil-specific parameter |
| Half life for degradation in soil at 20°C | DegT50 | days | Substance-specific parameter |

Step 3: calculation of the maximum concentration in soil

***Formula 6:***

$$C_{T,peak} = C_{T,ini} + C_{T,plateau}$$

With:

**Table 7:** Parameters in formula $C_{T,peak}$

| | **Symbol** | **Unit** | **Default values/Input** |
|---|---|---|---|
| **Parameter** | | | |
| Initial total concentration in soil | $C_{T,ini}$ | $mg.kg^{-1}$ | Step 1 |
| Background concentration in soil just before next application | $C_{T,plateau}$ | mg.kg-1 | Step 2 |
| Maximum total concentration in soil | $C_{T,peak}$ | $mg.kg^{-1}$ | Formula 6 |

Step 4: calculation of the maximum concentration in liquid phase

***Formula 7:***

$$C_{L,peak} = \frac{C_{T,peak}}{\theta / \rho + f_{om} K_{om}}$$

With:

**Table 8:** Parameters in formula $C_{L,peak}$

| | Symbol | Unit | Default values/Input |
|---|---|---|---|
| **Parameter** | | | |
| Maximum total concentration in soil | $C_{T,peak}$ | $mg.kg^{-1}$ | Formula 3 |
| Volumetric water content | $\theta$ | $m^3.m^{-3}$ | Soil-specific parameter |
| Dry bulk density | $\rho$ | $kg\ L^{-1}$ | Soil-specific parameter |
| Organic matter content | $f_{om}$ | $kg.kg^{-1}$ | Soil-specific parameter |
| Organic matter/water distribution coefficient | $K_{om}$ | $L.kg^{-1}$ | Substance-specific parameter |
| Maximum liquid concentration in soil | $C_{L,peak}$ | $mg.L^{-1}$ | Formula 7 |

Step 5: calculation of the TWA concentration in total soil

***Formula 10:***

$$C_{T,TWA} = \frac{C_{T,peak}}{t_{avg}\ f_T\ k_{ref}}\left[1 - \exp\left(-f_T\ k_{ref}\ t_{avg}\right)\right]$$

The TWA concentration in the liquid phase, $C_{L,TWA}$, is calculated according the formula 10 but with $C_{L,peak}$ instead of $C_{T,peak}$.

With:

**Table 9:** Parameters in formula $C_{T,TWA}$

| | Symbol | Unit | Default values/Input |
|---|---|---|---|
| **Parameter** | | | |
| Time weighted average (TWA) total concentration in soil | $C_{T,TWA}$ | $mg.kg^{-1}$ | Formula 10 |
| Maximum total concentration in soil | $C_{T,peak}$ | $mg.kg^{-1}$ | Step 3 |
| Time period since application time over which concentrations | $t_{avg}$ | days | 7; 14; 21; 28; 56 days |

| | | | |
|---|---|---|---|
| are averaged | | | |
| Correction factor for temperature | $f_T$ | | Formula 4 |
| Degradation rate coefficient at reference temperature | $k_{ref}$ | $days^{-1}$ | Step 2 |
| Maximum liquid concentration in soil | $C_{L,peak}$ | $mg.L^{-1}$ | Step 5 |
| Time weighted average (TWA) liquid concentration in soil | $C_{L,TWA}$ | $mg.L^{-1}$ | Formula 10 |

Step 6: calculation for metabolites

Using the same formulas but with an equivalent annual application rate in Formula 1:

***Formula 13:***

$$A_{met,1} = F_{f,1\_p} \frac{M_{met,1}}{M_{parent}} A$$

***Formula 14:***

$$A_{met,2} = F_{f,1\_p} F_{f,2\_1} \frac{M_{met,2}}{M_{parent}} A$$

With:

**Table 10:** Parameters in formula $A_{met,1}$ and $A_{met,2}$

| | Symbol | Unit | Default values/Input |
|---|---|---|---|
| **Parameter** | | | |
| Formation fraction for the first metabolite | $F_{f,1\_p}$ | | Substance-specific parameter |
| Formation fraction for the second metabolite | $F_{f,2\_p}$ | | Substance-specific parameter |
| Molar mass of the first metabolite | $M_{met,1}$ | $g.mol^{-1}$ | Substance-specific parameter |

| | | | |
|---|---|---|---|
| Molar mass of the second metabolite | $M_{met,2}$ | $g.mol^{-1}$ | Substance-specific parameter |
| Molar mass of the parent substance | $M_{parent}$ | $g.mol^{-1}$ | Substance-specific parameter |
| Equivalent annual application rate first metabolite | $A_{met,1}$ | $kg.ha^{-1}$ | Formula 13 |
| Annual application rate | A | $kg.ha^{-1}$ | Input field tab Substances |
| Equivalent annual application rate second metabolite | $A_{met,2}$ | $kg.ha^{-1}$ | Formula 14 |

### 8.2.2. Applying scenario adjustment factor and model adjustment factor

#### 8.2.2.1. Scenario adjustment factors

In this manual crop extrapolation factor is replaced by the term scenario adjustment factor following the advice from the EFSA WG on PECs in soil.

Scenario adjustment factors are used to account for the use of a virtual target croup group instead of the actual area where a target crop or crop group is cultivated. The virtual target crop group is defined as the spatial statistical population of all annual crops within each regulatory zone. Scenario adjustment factors are derived for the different endpoints and regulatory zones and for either CAPRI crops or other crops.

The opinion advises to use the maximum values for each endpoint and regulatory zones (third and fifth column in the following tables). The scenario adjustment factors should be applied in step 3, step 4 and step 5 of the calculation.

**Table 11:** Scenario adjustment factors for CAPRI crops

| | $C_{T,peak}$ [a] | $C_{L,peak}$ [a] |
|---|---|---|
| **Zone** | | |
| North | 3.0 | 2.0 |
| Centre | 2.0 | 1.5 |
| South | 2.0 | 1.5 |

(a) rounded up at 0.5 steps

#### 8.2.2.2. Model adjustment factors

Model adjustment factors are introduced to account for the use of a simple analytical model instead of a more detailed process-based numeric model.

The recommendation of the EFSA WG on PECs for the model adjustment factor (Fmo) in soil according to email from EFSA to VITO dated 2 September 2013 is as follows:

- Model adjustment factor $F_{mo}$ = 2.0 for concentrations in total soil
- Model adjustment factor $F_{mo}$ = 4.0 for concentration in pore water

These are used for the parent substances and the metabolites. The same model adjustment factors are applied for parent substances and metabolites.

The model adjustment factors should be applied in step 5 of the calculation.

$$C_{Y,cal} = F_{mo}\ C_Y$$

$C_{y,cal}$ is the calibrated concentration, $C_y$ is the uncalibrated concentration.

This formula should be used for $C_{T,peak}$, $C_{L,\ peak}$, $C_{T,TWA}$ and $C_{L,TWA}$ (Step 3, step 4 and step 5 of the calculations)

## 8.3. TIER-1 overview

The overview tab shows the configured settings and the zone and endpoint dependent parameter values that will be used in the calculations.All parameters are not editable.

Next table gives an overview of the parameters dependant on the zone and endpoint

**Table 12:** Parameters dependant on the zone and endpoint

| | Symbol | Unit |
|---|---|---|
| **Parameter** | | |
| Temperature $T_{Arit}$ | $T_{Arit}$ | K |
| Temperature $T_{Arr}$ | $T_{Arr}$ | K |
| Volumetric water content | $\theta$ | $m^3\ m^{-3}$ |
| Dry bulk density | $\rho$ | $Kg\ L^{-1}$ |
| Organic matter content | $f_{om}$ | $kg.kg^{-1}$ |

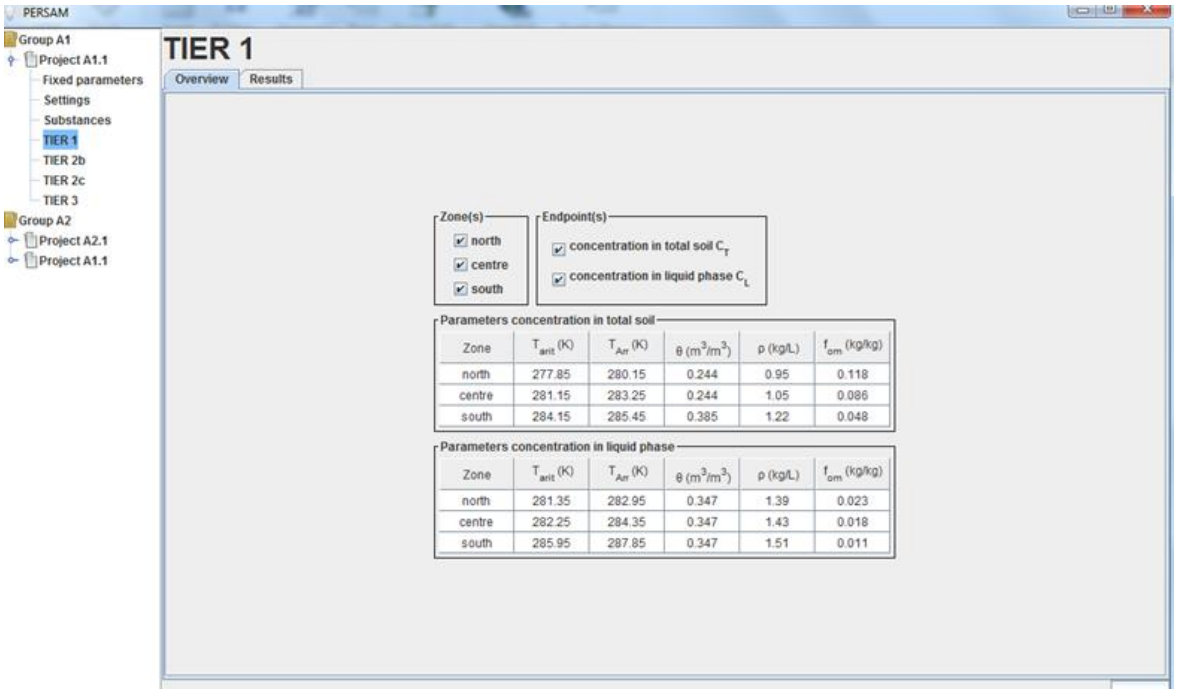



**Figure 47: TIER-1 overview tab**

### 8.4. TIER-1 results

The user can start the calculations and view the results.

1. Click on 'Start'
2. The calculations start and following dialog box appears.

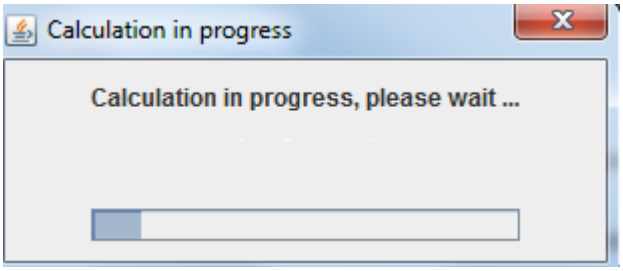



**Figure 48: Dialog Calculation in progress**

3. The results appear on the screen. Select a substance in the Substance tree to view the results.

**Other functionalities:**

- Delete the results
- Create a PDF report of the results
- Export the results to a CSV file

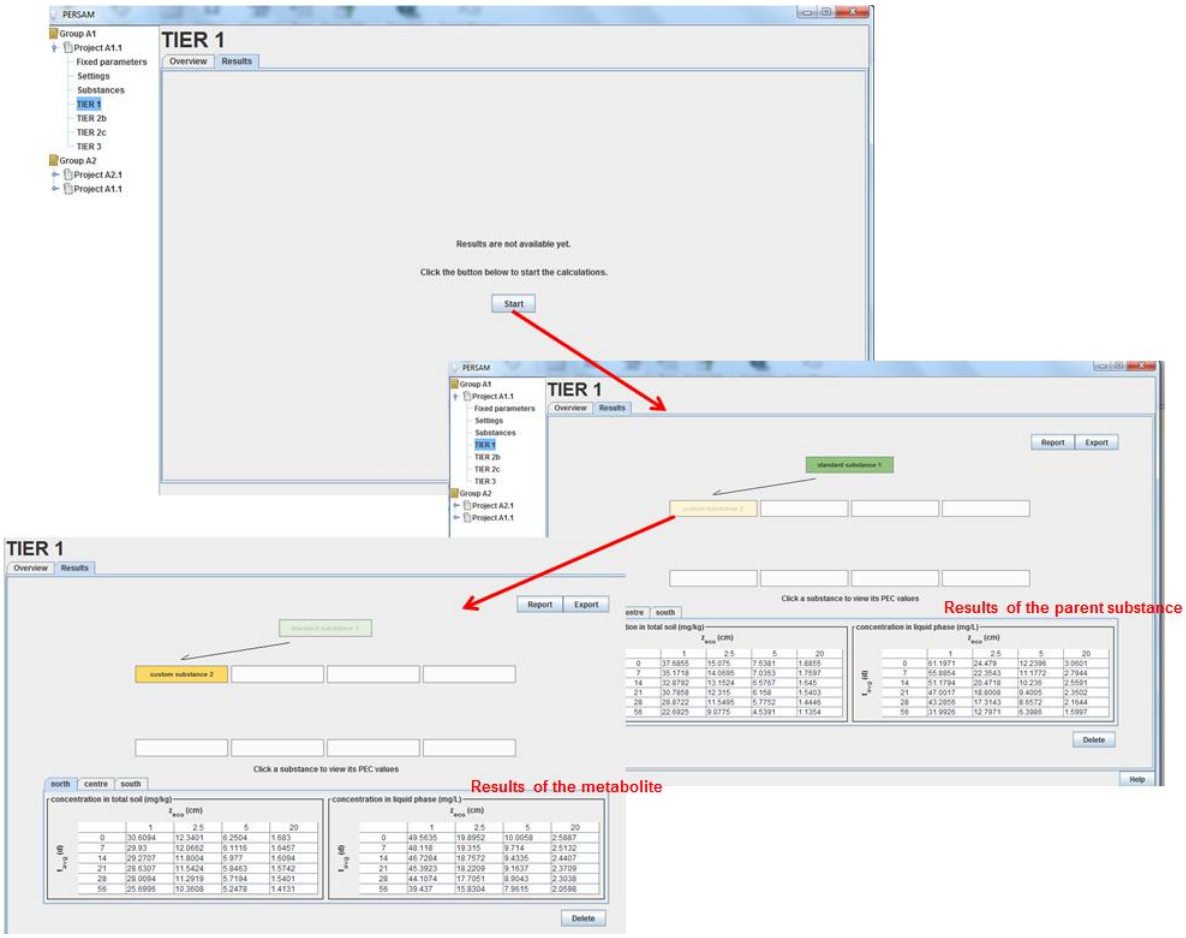



**Figure 49: Results of TIER-1**

# 9. TIER-2B

TIER-2B is used to calculate the 95$^{th}$-percentile PECs. Instead of one scenario for each regulatory zone and endpoint (total concentration or pore water concentration), the model is applied to all 1 km by 1 km grid cells (combination of soil moisture content, soil bulk density, soil organic matter, temperature) where the target crop or crop group is present. In this tier, relationships between $K_{om}$ and DegT50 and soil properties can be incorporated in the calculations. The output is the statistical distribution of concentrations for the considered endpoint and averaging depth from which the overall 95$^{th}$ percentile can be selected. In TIER-2B, it suffices to calculate the 95$^{th}$ spatial percentile of the PEC of the required type of concentration.

The TIER-2B section is shown in following figure.

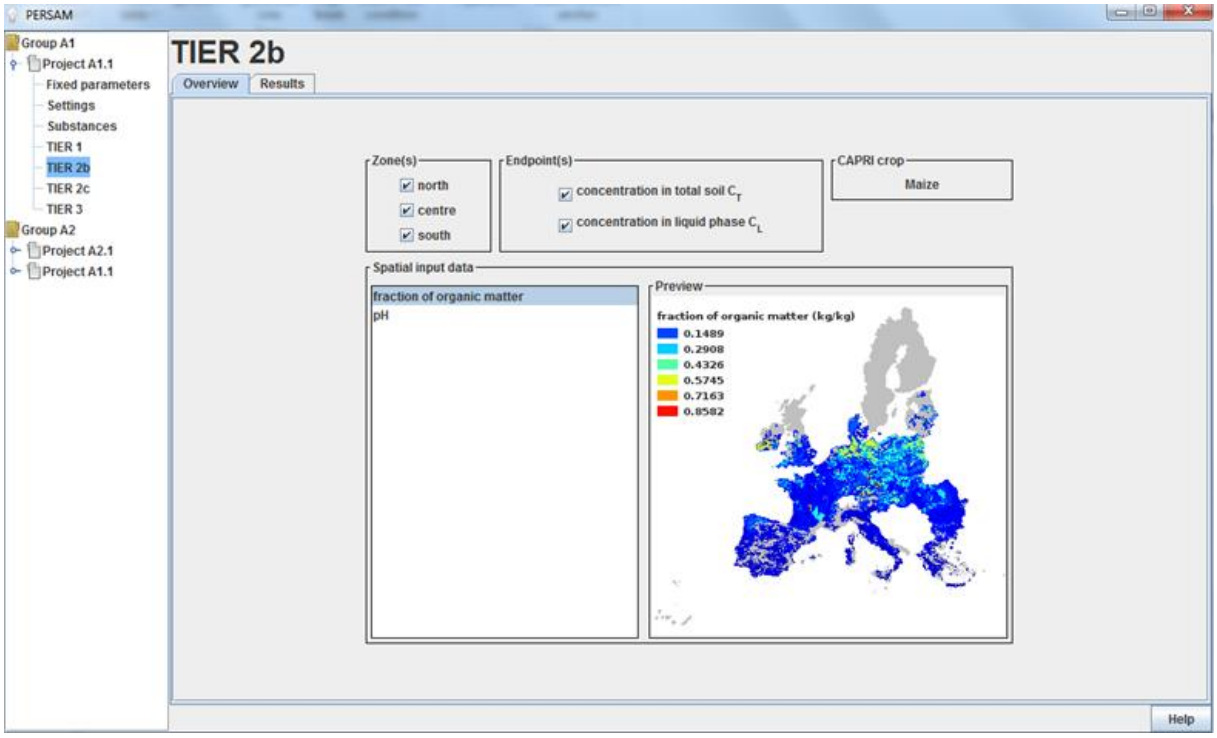



**Figure 50: TIER-2B section**

## 9.1. TIER-2B settings

TIER-2B settings for the calculation of the PEC values are:

- Zone(s) (see settings section)
- Endpoint(s) (see settings section)
- CAPRI crop (see settings section)
- Substances (parent & metabolites) (see substance section)

The user can define relationships between Kom, DegT50 and soil properties. (see Configure custom calculations )

## 9.2. TIER-2B calculations

The calculation for the 95the spatial percentile of the PEC with the simple analytical model is as follows:

- ✓ Apply the land-use mask of the annual crops (CAPRI crops) to all maps
- ✓ Check the underlying maps and eliminate pixels that have unrealistic properties (e.g. zero organic-matter contents)
- ✓ Based on the map of the relevant crop or crop group, create a map of the required type of concentration ($C_{L,peak}$ or $C_{T,peak}$ or any of the TWA averages) for the required ecotoxicological averaging depth ($z_{eco}$) and for the DegT50 – $K_{om}$ properties of this substance.
- ✓ Calculate from this concentration map the cumulative frequency distribution of PEC values. In this calculation the PEC of each 1x1km$^2$ pixel should get a weight that is proportional of the fraction of surface area grown with this crop or crop group.
- ✓ Take the 95$^{th}$ percentile PEC from this cumulative frequency distribution.

## 9.3. TIER-2B overview

The overview tab shows the configured settings and the spatial input data that will be used in the calculations.All parameters are not editable, the user can only select a spatial input data and preview the map.

The spatial input maps are:

- Fraction of organic matter
- pH

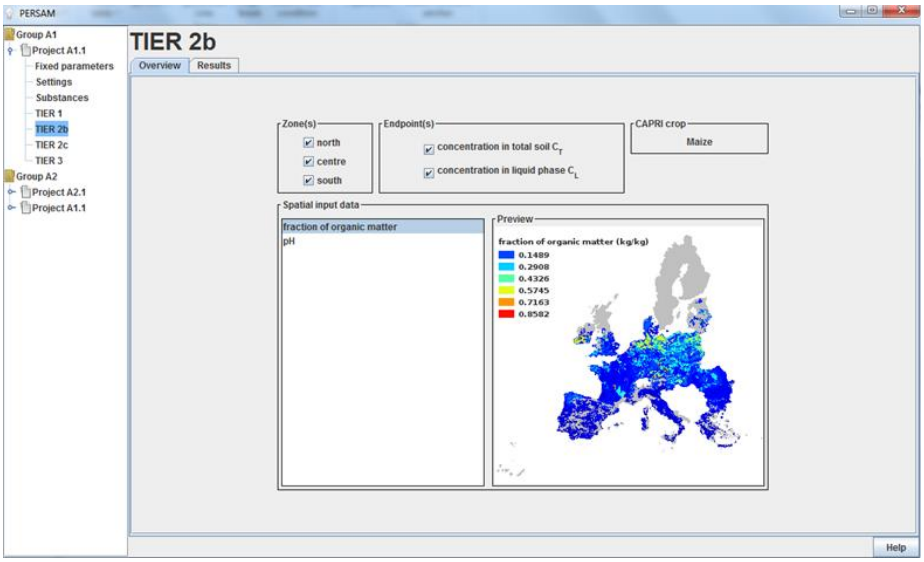


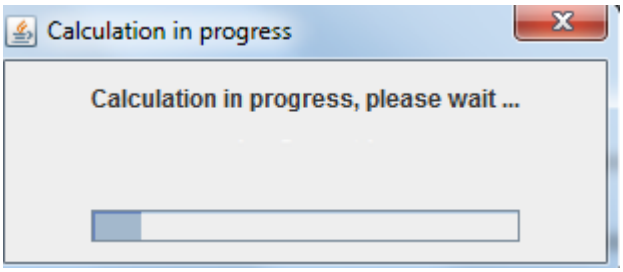

**Figure 51: TIER-2B overview tab**

## 9.4. TIER-2B results

The user can start the calculations and view the results.

1. Click on 'Start'

2. The calculations start and following dialog box appears.




3. The results appear on the screen. Select a substance in the Substance tree to view the results. The table contains a field for each combination of endpoint, ecotoxicological averaging depth and time window.

4. Click on a cell in the table to view extended results. A detail window appears containing the 95$^{th}$ spatial percentile of calculated PECs for the regulatory selected zone with the related cumulative distribution graph and map.

**Other functionalities:**

- Delete the results
- Create a PDF report of the results
- Export the results to a CSV file

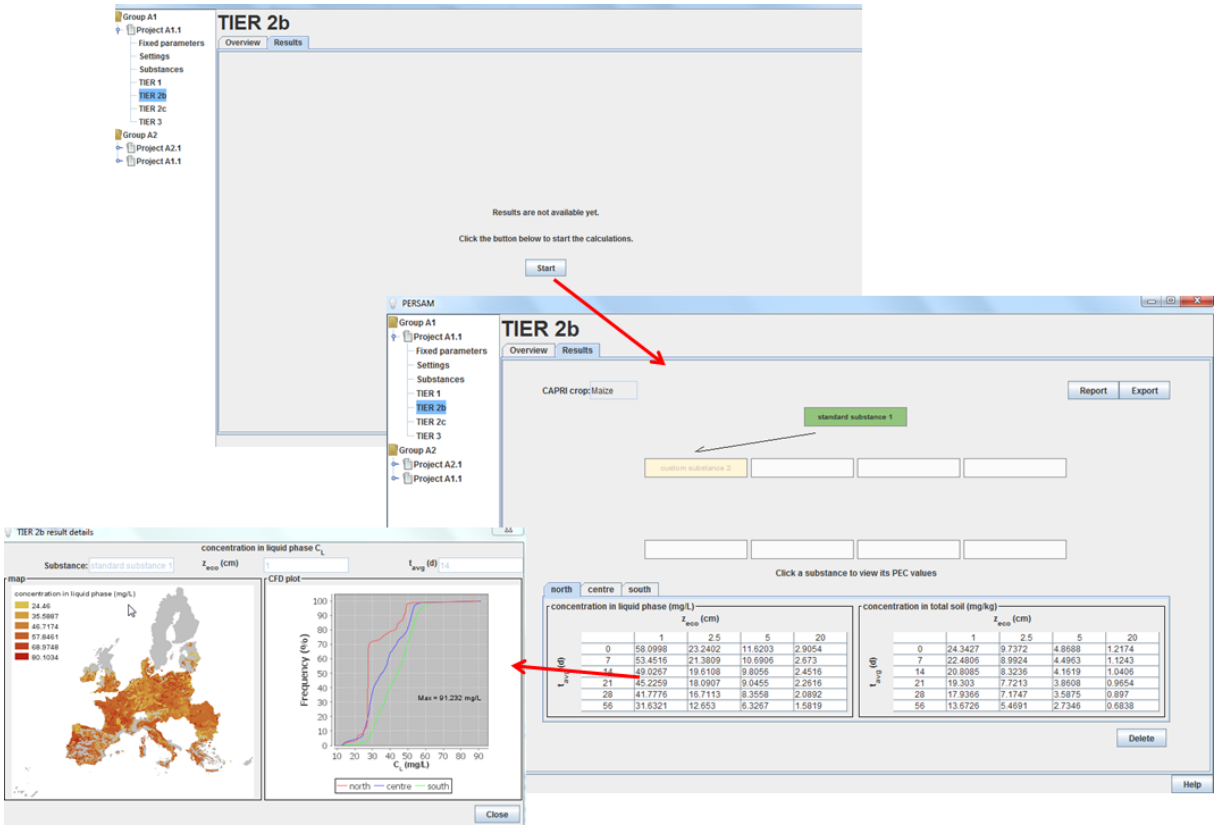



**Figure 52: results of TIER-2B**

## 10. TIER-2C

TIER-2C is almost analogue to TIER-2B, only that the user should define an extra parameter, the fraction that reached the soil $F_{soil,max}$, which he must retrieve from model calculations outside of this tool. TIER-2C can only be calculated on the condition the user first calculates TIER-2B.

The TIER-2C section is shown in following figure.

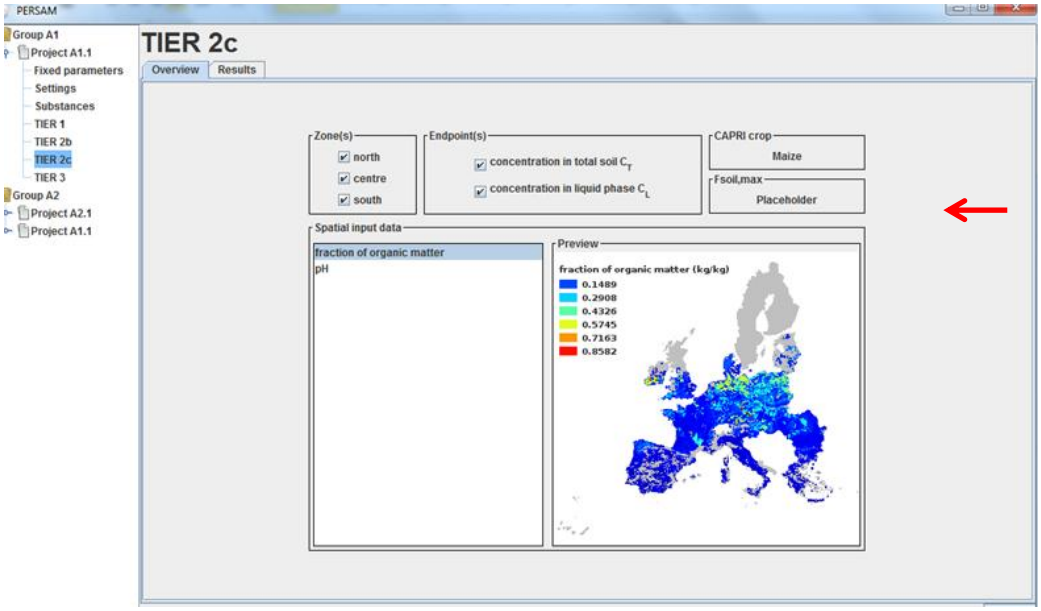



**Figure 53: TIER-2C section**

### 10.1. TIER-2C settings

TIER-2C settings for the calculation of the PEC values are:

- Zone(s) (see settings section)
- Endpoint(s) (see settings section)
- CAPRI crop (see settings section)
- Substances (parent & metabolites) (see substance section)
- Fraction that reached the soil ($F_{soil,max}$) (see settings section)

The user can define relationships between Kom, DegT50 and soil properties. (see Configure custom calculations )

## 10.2. TIER-2C calculations

TIER-2C can only be calculated on the condition the user first calculates TIER-2B

The calculations of TIER-2C are based on the calculations of TIER-2B (see TIER-2B calculations) The relationship between TIER-2B and TIER-2C is following formula:

$$PEC_{2C} = F_{soil,max} PEC_{2B}$$

## 10.3. TIER-2C overview

The overview tab shows the configured settings and the spatial input data that will be used in the calculations. All parameters are not editable, the user can only select a spatial input data and preview the map.

The spatial input maps are:

- Fraction of organic matter
- pH

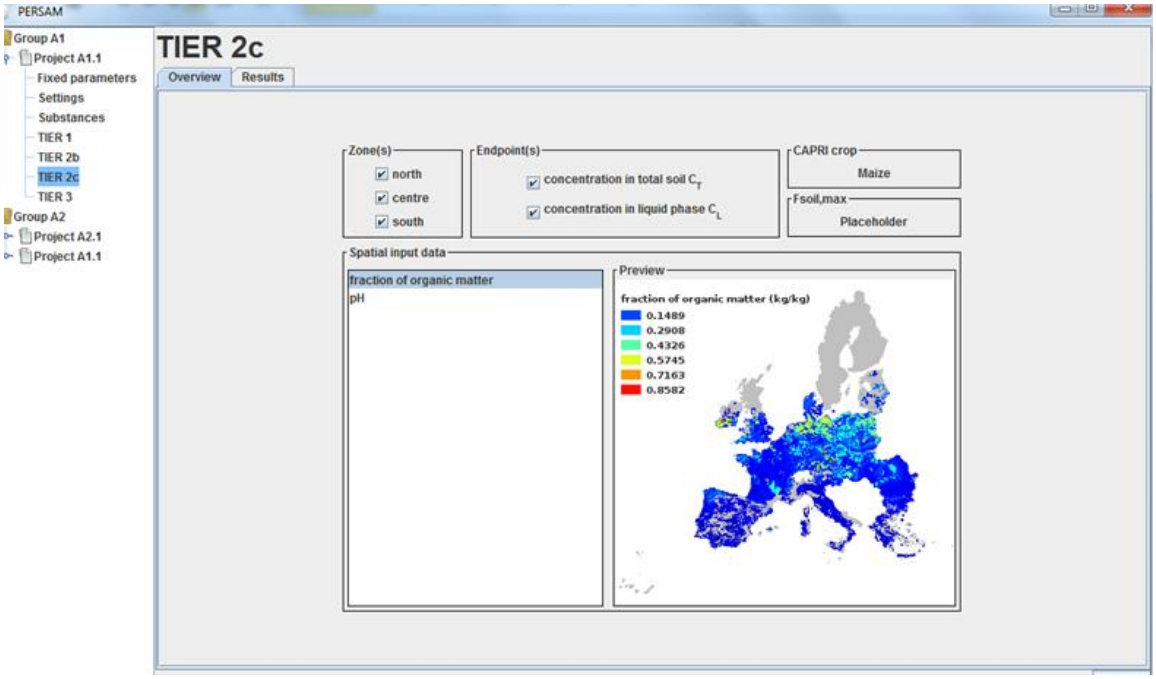
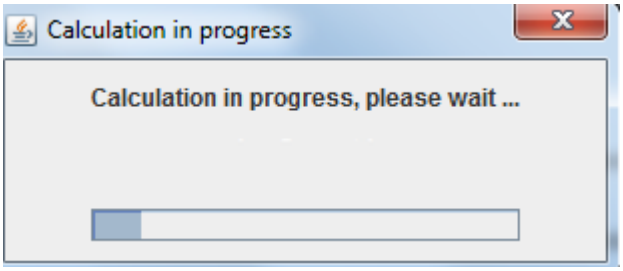



**Figure 54: TIER-2C overview tab**

### 10.4. TIER-2C results

The user can start the calculations and view the results.

1. Click on 'Start'
2. The calculations start and following dialog box appears.




3. The results appear on the screen. Select a substance in the Substance tree to view the results. The table contains a field for each combination of endpoint, ecotoxicological averaging depth and time window.
4. Click on a cell in the table to view extended results. A detail window appears containing the 95$^{th}$ spatial percentile of calculated PECs for the regulatory selected zone with the related cumulative distribution graph and map

**Other functionalities:**

- Delete the results
- Create a PDF report of the results
- Export the results to a CSV file

## 11. TIER-3

TIER-3 is designed to select the grid cell including the scenario properties corresponding to the 95$^{th}$-percentile PEC as needed for the scenario development of TIER-3. The PERSAM software provides the model parameters for the scenario corresponding to a 95% vulnerability scenario. The actual calculation of the scenario is to be done with a numerical model outside of PERSAM.

The TIER-2C section is shown in following figure.

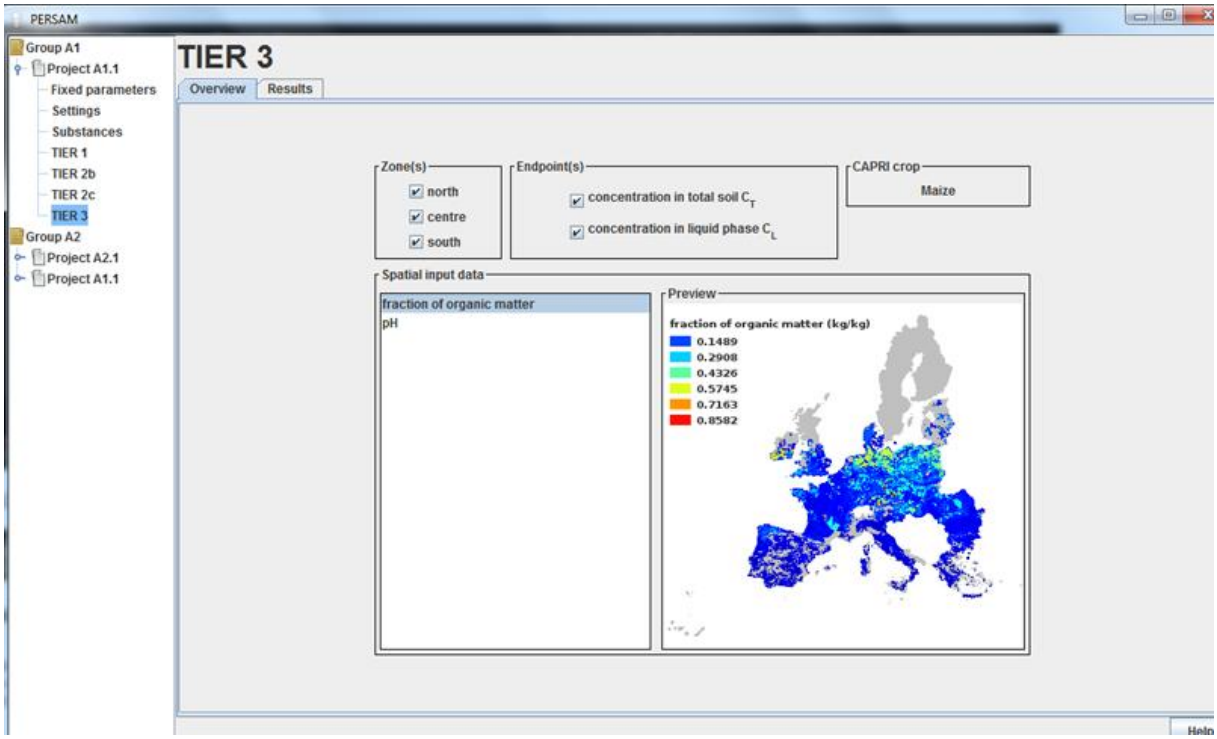



**Figure 55: TIER-3 section**

### 11.1. TIER-3 settings

TIER-3 settings for the calculation of the PEC values are:

- Zone(s) (see settings section)
- Endpoint(s) (see settings section)
- CAPRI crop (see settings section)
- Substances (parent & metabolites) (see substance section)

## 11.2. TIER-3 calculations

TIER-3 uses the same analytical model as TIER-2B but for scenario selection rather than for risk evaluation. The analytical model is applied for each 1 km by 1 km grid cell where the target crop or crop group is present for the different endpoints and averaging depths. No scenario adjustment or model adjustment factors are applied. The maps of calculated concentrations are converted to vulnerability maps by ranking the concentrations and assigning to each grid cell a vulnerability index corresponding to the concentration and the fraction of surface area grown with this crop or crop group. The grid cell which corresponds to a 95% vulnerability can then be selected and used for the scenario development for simulation with a numerical model in TIER-3.

The Tier-3 scenario is selected with the simple analytical model using the procedure to find the scenario for the 95$^{th}$ spatial percentile:

- ✓ Apply the land-use mask of the annual crops to all maps.
- ✓ Based on the map of the relevant crop or crop group, create individual maps for each endpoint (e.g. $C_{L,peak}$ or $C_{T,\,peak}$ or any of the TWA concentrations for $z_{eco}$ of 1, 2.5, 5 or 20 cm) and for the $DegT50$ - $K_{om}$ properties of this substance; so this gives only one map that applies only to the type of concentration considered in one of the regulatory zones.
- ✓ Transform the concentration map into a vulnerability map by assigning to each grid cell the percentile corresponding to its concentration. In the calculation of this percentile, each 1×1 km$_2$ pixel should get a weight that is proportional to the fraction of surface area grown with this crop or crop group.
- ✓ Select from the vulnerability map the grid cell with the percentile that is closest to 95%.
- ✓ Use this grid cell to parameterize the scenario.

## 11.3. TIER-3 overview

The overview tab shows the configured settings and the spatial input data that will be used in the calculations. All parameters are not editable, the user can only select a spatial input data and preview the map.

The spatial input maps are:

- Fraction of organic matter
- pH

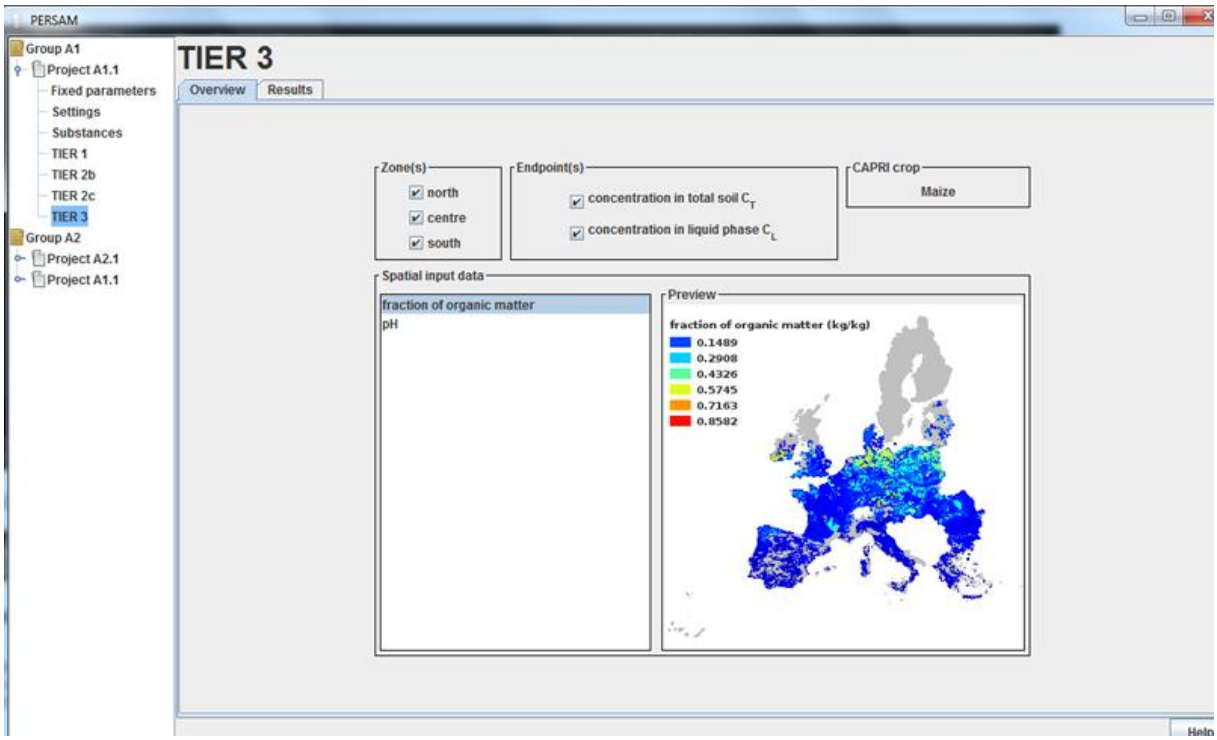



**Figure 56: TIER-3 overview tab**

## 11.4. TIER-3 results

The user can start the calculations and view the results.

1. Go to the 'Results' tab
2. Select a substance in the Substance tree to view the results. The results tab of TIER-3 contains a table with the green cells which indicates whether there results are available.
3. Click on a particular cell (a combination of ecotoxicological averaging depth, time window and endpoint) and there will appear a result window containing the model parameters for the TIER-3 scenario and the vulnerability map showing the calculated vulnerability indices and the location of the grid cell corresponding to a 95% vulnerability

**Other functionalities:**

- Delete the results
- Create a PDF report of the results
- Export the results to a CSV file

  The selected scenario can be exported out side the PERSAM tool to a numerical model for a refined exposure assessment.

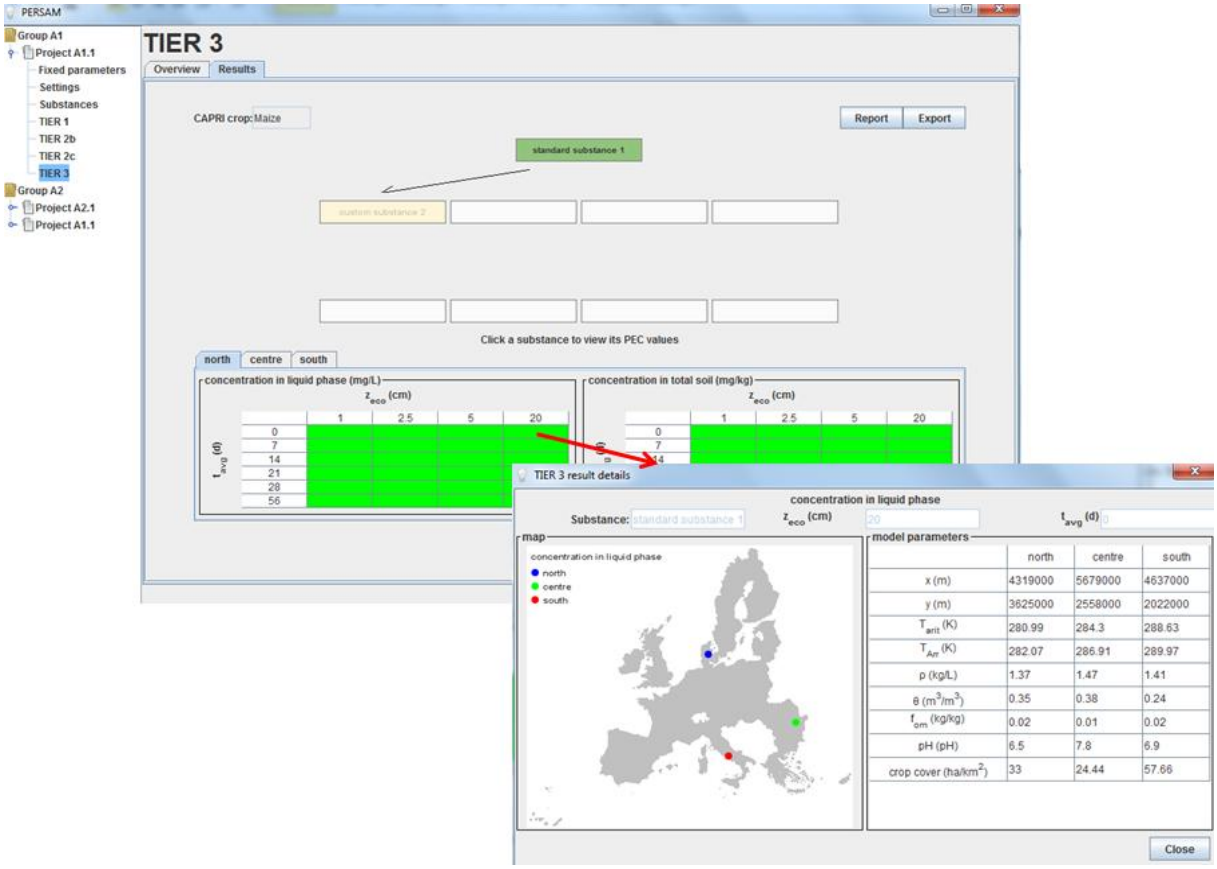



**Figure 57: Results of TIER-3**

The x and y model parameters in the TIER-3 results window indicate the coordinates of the lower left corner of the grid cell.
Since the lower left corner of the grid is defined as x = 1500000, y = 900000, and the cell size is defined as 1000, the coordinates of the lower left corner of each cell in the grid are pluralities of 1000.

## 12. Reporting and export results

PERSAM generates PDF reports of the results of TIER-1, TIER-2B, TIER-2C and TIER-3 and provides the functionality to export the results to a CSV file.

### 12.1. Reporting

PERSAM generates PDF reports of the results of TIER-1, TIER-2B, TIER-2C and TIER-3.

1. Go to the results tab of a particular TIER
2. Click on 'Report'
3. The popup window 'Generate report' appears. Give the location where you want to save the PDF report
4. Click on 'Save'
   PERSAM generates and opens the PDF report.

**Remark:** You can use the information of the PDF report in other WORD documents, by selecting the text in the PDF report and copy/paste to the word document.

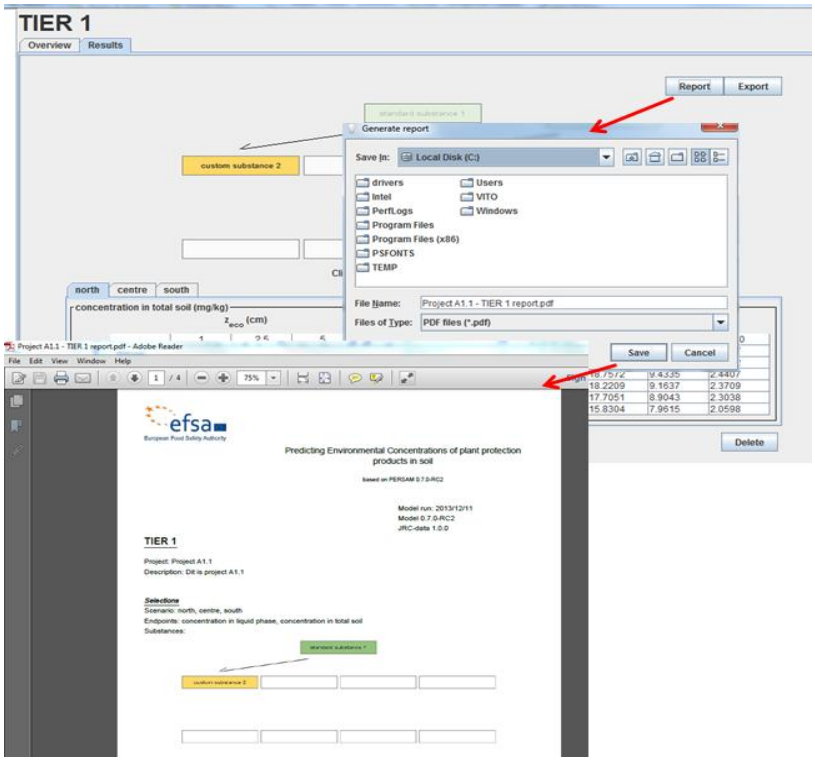



**Figure 58: Reporting**

## 12.2. Export results

PERSAM provides the functionality to export the results of TIER-1, TIER-2B, TIER-2C and TIER-3 to a CVS file.

1. Go to the results tab of a particular TIER
2. Click on 'Export'
3. The popup window 'Export' appears. Give the location and the file name for the export file.
4. Click on 'Export'
   PERSAM exports the results to the CSV file.

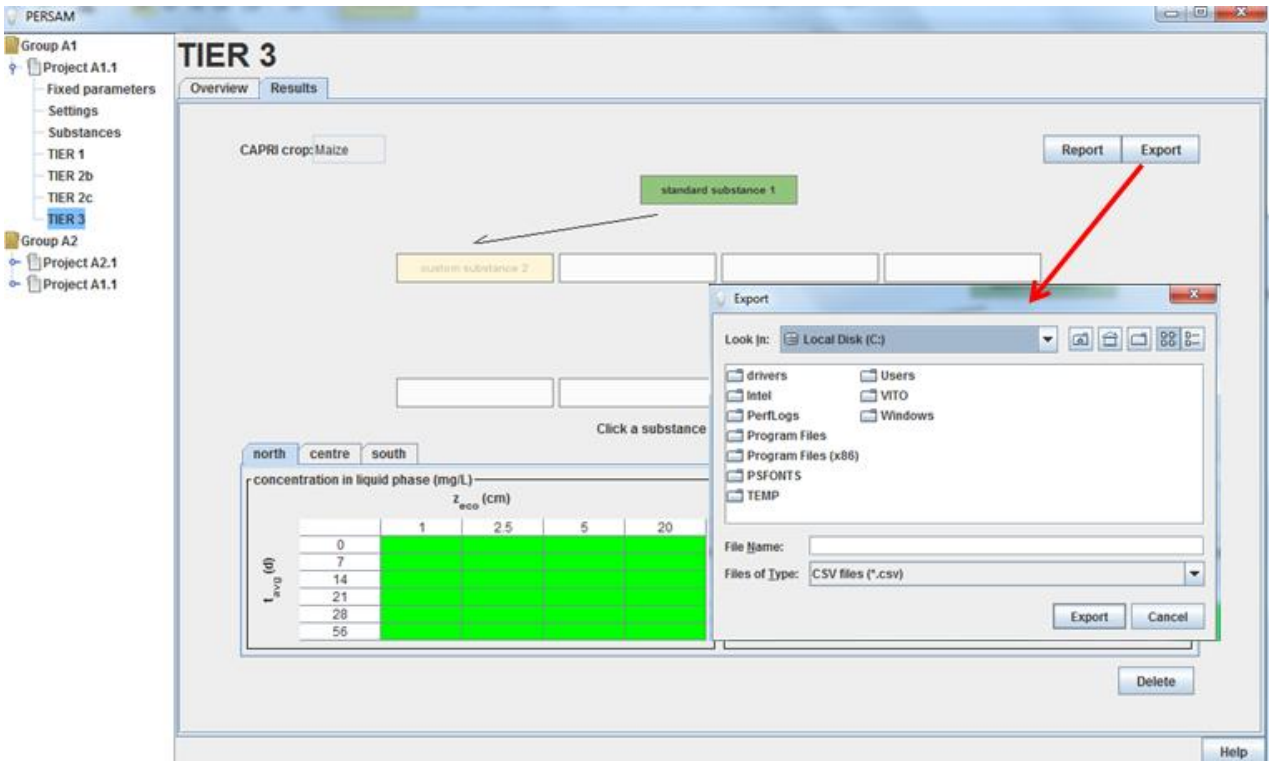



**Figure 59: Export results**

# 13. Additional information

This section contains additional information such as:

- CAPRI Crops
- EFSA Spatial version

## 13.1. CAPRI Crops

Next table contains the CAPRI crop list.

**Table 13:** CAPRI crops

| Crops |
|---|
| Barley |
| Common wheat |
| Durum wheat |
| Fallow |
| Floriculture and flower bulbs |
| Maize |
| Oats |
| Oilseed rapes |
| Other annual crops |
| Other cereals |
| Other fodder on arable land |
| Other fresh vegetables |
| Other non-permanent industrial crops |
| Other root crops |
| Potatoes |
| Pulses |
| Rye |
| Soyabeans |
| Sugar beets |
| Sunflowers |
| Texture crops |
| Tobacco |
| Tomatoes |

### 13.2. EFSA Spatial data

The EFSA spatial data set version 1.1 includes following maps:

**Table 14:** EFSA Spatial data version 1.1

| Title | Area covered |
|---|---|
| **General data** | |
| EFSA Data Mask | EU27 |
| EFSA European Union Cover | EU27 |
| EFSA EU Regulatory Zones | EU27 |
| EFSA Corine Land Cover Data | EU27 |
| EFSA Generalized Land Use Map | EU27 |
| FOCUS Zones | EU27 |
| **Meteorological data** | |
| Mean monthly temperature, January | EU27 |
| Mean monthly temperature, February | EU27 |
| Mean monthly temperature, March | EU27 |
| Mean monthly temperature, April | EU27 |
| Mean monthly temperature, May | EU27 |
| Mean monthly temperature, June | EU27 |
| Mean monthly temperature, July | EU27 |
| Mean monthly temperature, August | EU27 |
| Mean monthly temperature, September | EU27 |
| Mean monthly temperature, October | EU27 |
| Mean monthly temperature, November | EU27 |
| Mean monthly temperature, December | EU27 |
| Annual mean temperature | EU27 |
| Arrhenius Weighted Mean Annual Temperature | EU27 |
| Mean monthly precipitation sum,January | EU27 |
| Mean monthly precipitation sum,February | EU27 |
| Mean monthly precipitation sum, March | EU27 |
| Mean monthly precipitation sum, April | EU27 |
| Mean monthly precipitation sum, May | EU27 |
| Mean monthly precipitation sum, June | EU27 |
| Mean monthly precipitation sum, July | EU27 |
| Mean monthly precipitation sum, August | EU27 |
| Mean monthly precipitation sum, September | EU27 |
| Mean monthly precipitation sum, October | EU27 |
| Mean monthly precipitation sum,November | EU27 |

| | |
|---|---|
| Mean monthly precipitation sum,December | EU27 |
| Annual mean precipitation sum | EU27 |
| **Soil data** | |
| Topsoil Organic Matter content | EU27 |
| Topsoil pH | EU27 |
| Topsoil Bulk Density | EU27 |
| Topsoil Texture Class | EU27 |
| Topsoil Water Content at Field Capacity | EU27 |
| **CAPRI2000 Crop Data** | |
| EFSA-CAPRI Common Mask | EU25 |
| EFSA-CAPRI Barley | EU25 |
| EFSA-CAPRI Common wheat | EU25 |
| EFSA-CAPRI Durum wheat | EU25 |
| EFSA-CAPRI Fallow land | EU25 |
| EFSA-CAPRI Floriculture | EU25 |
| EFSA-CAPRI Maize | EU25 |
| EFSA-CAPRI Oats | EU25 |
| EFSA-CAPRI Other cereals | EU25 |
| EFSA-CAPRI Other annual crops | EU25 |
| EFSA-CAPRI Fodder other on arable land | EU25 |
| EFSA-CAPRI Other non permanent industrial crops | EU25 |
| EFSA-CAPRI Other root crops | EU25 |
| EFSA-CAPRI Other fresh vegetables | EU25 |
| EFSA_CAPRI Potatoes | EU25 |
| EFSA-CAPRI Dry pulses | EU25 |
| EFSA-CAPRI Rape and turnip rape | EU25 |
| EFSA-CAPRI Rye | EU25 |
| EFSA-CAPRI Soya | EU25 |
| EFSA-CAPRI Sugar beet | EU25 |
| EFSA-CAPRI Sunflower | EU25 |
| EFSA-CAPRI Fibre and oleaginous crops | EU25 |
| EFSA-CAPRI Tobacco | EU25 |
| EFSA-CAPRI Tomatoes | EU25 |

*EU25: E27 without Malta, Cyprus and some smaller areas*

The EFSA spatial data can be found on the website of the JRC soil portal http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/

## 14. Troubleshooting and Helpdesk

Troubleshooting during the installation procedure:

- ***There is not enough disk space:***
  The software requires 1.2GB disk space for the installation.
  It is advisable to provide 10 GB of free disk space to comfortably work with PERSAM for the sake of the required temporary disk space

- ***User rights:***
  The user should have write rights in the user directory and in the directory where you install the PERSAM software.

Problem reporting:

***Following information is required for reporting the problem***:

- What is your operating system and version number?
- Where is the PERSAM directory located: on the disk of your pc or on a network disk?
- Do you have administrator rights on your pc? If not, what rights do you have?
- Please, give a detailed description of the different steps you've done before the problem popped up.
- Deliver also the log file 'PERSAM.log', which you can find in the directory where you've installed the PERSAM software.

*If you have problems with the installation or use of the PERSAM software, please send an email on the JRC soil portal. For software related issues your email will be forwarded to VITO.*

## REFERENCES

EFSA, 2010. European Food Safety Authority; Selection of Scenarios for Exposure of Soil Organisms to Plant Protection Products. EFSA Journal 2010;8(6):1642 [82pp.]. doi:10.2903/j.efsa.2010.1642.

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EFSA, 2012b. EFSA Panel on Plant Protection Products and their Residues; Scientific Opinion on the science behind the guidance for scenario selection and scenario parameterisation for predicting environmental concentrations in soil. EFSA Journal 2012;10(2):2562. [76 pp.] doi:10.2903/j.efsa.2012.2562.

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# APPENDICES

## A. CAPRI CROPS[1]

| Crops |
|---|
| Barley |
| Common wheat |
| Durum wheat |
| Fallow |
| Floriculture and flower bulbs |
| Maize |
| Oats |
| Oilseed rapes |
| Other annual crops |
| Other cereals |
| Other fodder on arable land |
| Other fresh vegetables |
| Other non-permanent industrial crops |
| Other root crops |
| Potatoes |
| Pulses |
| Rye |
| Soyabeans |
| Sugar beets |
| Sunflowers |
| Texture crops |
| Tobacco |
| Tomatoes |

**Figure 60: Capri crops**

[1] See Parameterisation of scenarios for exposure of soil organisms, EFSA 2010

## B. SOIL-SPECIFIC PARAMETERS[2]

### Total concentration in soil

| Zone | Country in which scenario is located | $T_{arit}$ (°C) | $T_{Arr}$ (°C) | Texture | Volume fraction of water, $\theta$ ($m^3$ $m^{-3}$) | Dry bulk density, $\rho$ (kg $L^{-1}$) | $f_{om}$ (%) |
|---|---|---|---|---|---|---|---|
| North | Estonia | 4.7 | 7.0 | Coarse | 0.244 | 0.95 | 11.8 |
| Centre | Germany | 8.0 | 10.1 | Coarse | 0.244 | 1.05 | 8.6 |
| South | France | 11.0 | 12.3 | Medium fine | 0.385 | 1.22 | 4.8 |

### Concentration in liquid phase

| Zone | Country in which scenario is located | $T_{arit}$ (°C) | $T_{Arr}$ (°C) | Texture | Volume fraction of water, $\theta$ ($m^3$ $m^{-3}$) | Dry bulk density, $\rho$ (kg $L^{-1}$) | $f_{om}$ (%) | $\rho f_{om}$ (kg $L^{-1}$) |
|---|---|---|---|---|---|---|---|---|
| North | Denmark | 8.2 | 9.8 | Medium | 0.347 | 1.39 | 2.3 | 0.032 |
| Centre | Czech Rep. | 9.1 | 11.2 | Medium | 0.347 | 1.43 | 1.8 | 0.026 |
| South | Spain | 12.8 | 14.7 | Medium | 0.347 | 1.51 | 1.1 | 0.017 |

[2] See Scientific opinion, EFSA 2012b

## C. SUBSTANCE-SPECIFIC PARAMETERS[3]

| Number of example substance | *DegT50* (d) at 20°C and pF = 2 | $K_{om}$ (L kg$^{-1}$) |
|---|---|---|
| 1 | 10 | 10 |
| 2 | 31 | 10 |
| 3 | 10 | 31 |
| 4 | 31 | 31 |
| 5 | 100 | 31 |
| 6 | 10 | 100 |
| 7 | 31 | 100 |
| 8 | 100 | 100 |
| 9 | 316 | 100 |
| 10 | 10 | 316 |
| 11 | 31 | 316 |
| 12 | 100 | 316 |
| 13 | 316 | 316 |
| 14 | 1000 | 316 |
| 15 | 10 | 1000 |
| 16 | 31 | 1000 |
| 17 | 100 | 1000 |
| 18 | 316 | 1000 |
| 19 | 1000 | 1000 |

As molar mass M a value of 300 g mol-1 is used for the example substances

[3] See Parameterisation of scenarios for exposure of soil organisms, EFSA 2010

## ABBREVIATIONS

| | |
|---|---|
| CAPRI | Common Agricultural Policy Regionalised Impact model |
| $C_L$ | Liquid concentration in soil ($mg.L^{-1}$) |
| $C_T$ | Total concentration in soil ($mg.kg^{-1}$) |
| DegT50 | Half life for degradation in soil at 20°C (days) |
| $\rho$ | Dry bulk density ($kg.L^{-1}$) |
| EFSA | European Food Safety Authority |
| $f_{om}$ | Organic matter content ($kg.kg^{-1}$) |
| $F_{soil, max}$ | Max (fraction that reached the soil) |
| JRC | European Commission Joint Research Centre |
| $K_{om}$ | Organic matter/water distribution coefficient ($L.kg^{-1}$) |
| MRLs | Maximum Residue Levels |
| NA | Not available |
| PEC | Predicted Environmental Concentration |
| PPP | Plant Protection Products |
| PU | Pesticides Unit |
| SAM | Simple Analytical Model |
| $T_{Arit}$ | Arithmetic mean temperature (K) |
| $T_{Arr}$ | Arrhenius weighted average soil temperature (K) |
| TWA | Time weighted average |
| $\theta$ | Volumetric water content ($m^3.m^{-3}$) |