Software tool for calculating the predicted environmental concentrations (PEC) of plant protection products (PPP) in soil for annual crops:

Draft user manual v2.0.0

VITO NV

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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 Predicted Environmental concentrations

- ✓ 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,

- ✓ The refined scenario adjustment factor as needed for the calculation of the TIER-3A result from the TIER-2A PEC's, and

- ✓ To select the grid cell including the scenario properties corresponding to the 95th-percentile PEC as needed for the scenario development of TIER-3B

Following the responses from an EFSA public consultation on the draft of the EFSA guidance document on PECs in soil (EFSA, 2015) a negotiated procedure (NP/EFSA/PRAS/2015/01) was launched to improve the PERSAM software tool. This report has been amended as a result of this negotiated procedure.

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), and in the EFSA Guidance document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil (EFSA Journal 2015;13(4):4093).

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 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,

- ✓ The refined scenario adjustment factor as needed for the calculation of the TIER-3A result from the TIER-2A PEC's, and

- ✓ To select the grid cell including the scenario properties corresponding to the 95th-percentile PEC as needed for the scenario development of TIER-3B

Following the responses from an EFSA public consultation on the draft of the EFSA guidance document on PECs in soil (EFSA, 2015) a negotiated procedure (NP/EFSA/PRAS/2015/01) was launched to improve the PERSAM software tool. This report has been amended as a result of this negotiated procedure.

This report contains the user manual of Persistence in Soil Analytical Model (PERSAM) version 2.0.0.

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1. Introduction

1.1. Background and Terms of Reference as provided by the requestor

In EFSA, the Pesticides Unit and the Panel on Plant Protection Products and their Residues (PRAS) 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 computerised 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 under this procurement, 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.

On 2012 EFSA launched an Open Call for tenders - CFT/EFSA/PRAS/2012/03 to find a contractor for the development of software models for predicting environmental concentrations of plant protection products in soil.

The contract was awarded to the company VITO (BE) and was signed on the 12/11/2012. Detailed information on the tasks to be performed under the original direct contract is set out in annex 1 of the contract CFT/EFSA/PRAS/03/CT01.

Following a public consultation of the draft EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil from 10th July 2014 to 4th September 2014 a number of stakeholders made proposals on how to improve the PERSAM software. Further the EFSA WG PECs in soil identified through the preparation of the EFSA guidance and during the testing of the PERSAM tools a need for improvements of the software.

Following the responses from an EFSA public consultation on the draft of the EFSA guidance document on PECs in soil (EFSA, 2015) a negotiated procedure (NP/EFSA/PRAS/2015/01) was launched to improve the PERSAM software tool. This report has been amended as a result of this negotiated procedure.

This contract/grant was awarded by EFSA to:

Contractor: VITO NV
Contract: "Development of software models for predicting environmental concentrations of plant protection products in soil" additional services
Contract number: CFT/EFSA/PRAS/2012/03/CT01

1.2.   Interpretation of the Terms of Reference

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 (Question number: EFSA-Q-2012-00877, EFSA Journal 2015;13(4):4093. Doi: 10.2903/j.efsa.2015.4093).

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)
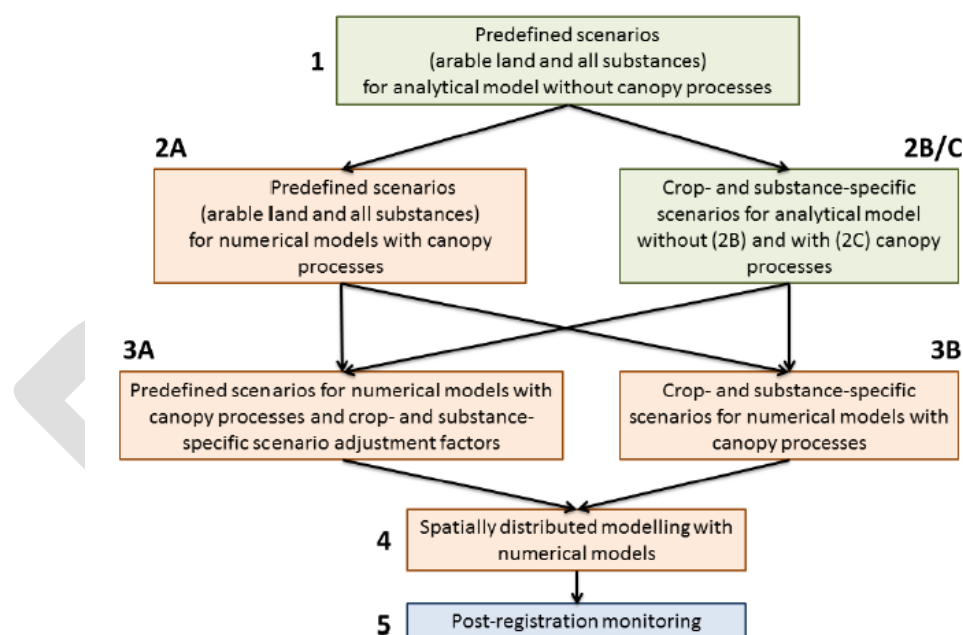
Figure 1: Tiered scheme for the exposure assessment of spray applications to annual crops under conventional or reduced tillage. The scheme applies to both the concentration in total soil and the concentration in pore water. Tiers 1, 2 and 3 are all based on one PEC for each of the regulatory zones, North, Central and South, and allow for one or multiple applications every one, two or three years. At Tiers 1 and 2B/C (green) the analytical model in the software tool PERSAM is used. At Tiers 2A, 3A, 3B and 4 (orange) modelling is carried out with numerical models

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 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,

- ✓ The refined scenario adjustment factor as needed for the calculation of the TIER-3A result from the TIER-2A PEC's, and

- ✓ To select the grid cell including the scenario properties corresponding to the 95th-percentile PEC as needed for the scenario development of TIER-3B

1.3.   What's new?

New features of PERSAM v2.0.0 are:

- ✓ Select FOCUS crops

- ✓ The option to limit Kom and DegT50 to user min and max values

- ✓ The option to generate a short report for one combination of Z_{eco} and t_{avg}

- ✓ The option for automatic report generation for full reports and short reports

- ✓ The user can enter application rate(s), application time and Fsoil for multiple applications

- ✓ TIER-3A

- ✓ Batch processing

2. Tutorial

Use the Tutorial for a quick start with the application.

- o *How can you start the PERSAM application?*
- o *How can you create a group?*
- o *How can you create a project?*
- o *How can you view the fixed parameters of the project?*
- o *How can you change the settings for the project?*
- o *How can you define a parent substance?*
- o *How can you define metabolites?*
- o *How can you define the relationship between the parent substance and a metabolite?*
- o *How can you perform the TIER-1 calculations?*
- o *How can you perform the TIER-2B calculations?*
- o *How can you perform the TIER-2C calculations?*
- o *How can you perform the TIER-3A calculations?*
- o *How can you perform the TIER-3B calculations?*
- o *How can you create a PDF report of the TIER-3B parameters?*
- o *Tips*

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
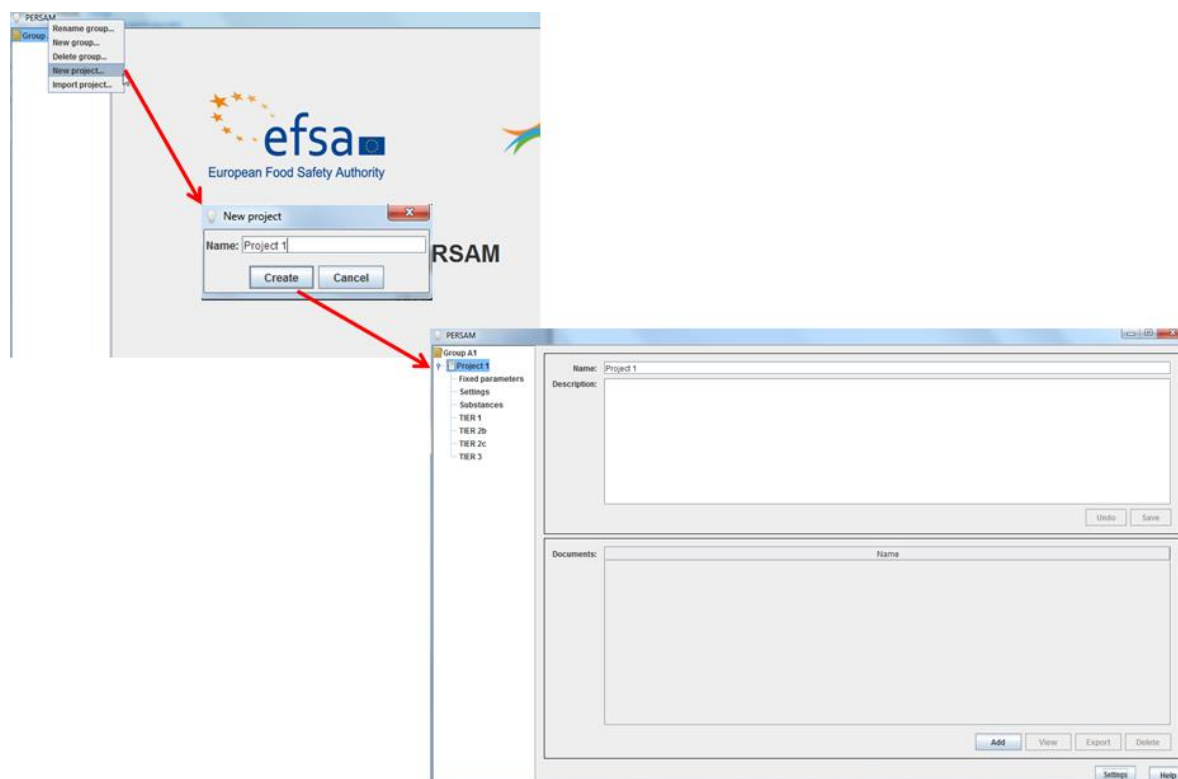
Figure 4: Project management – Create a new project

How can you view the fixed parameters of the project?

1. Go to the project tree
2. Select 'Fixed parameters'
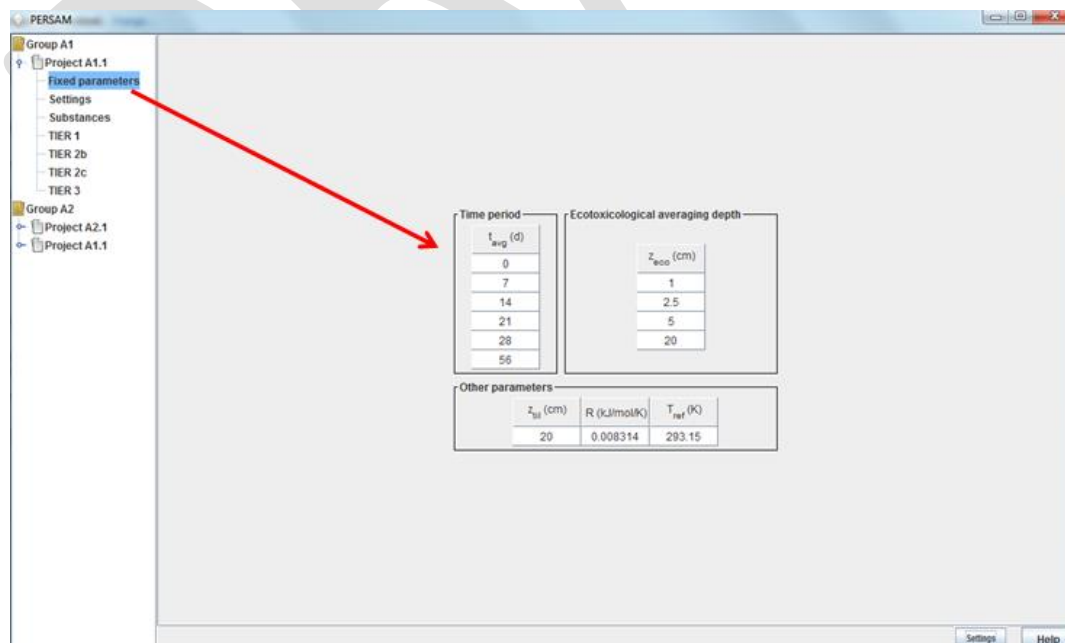
Figure 5: Fixed parameters

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 FOCUS crop (e.g. Maize) and click on 'Save'
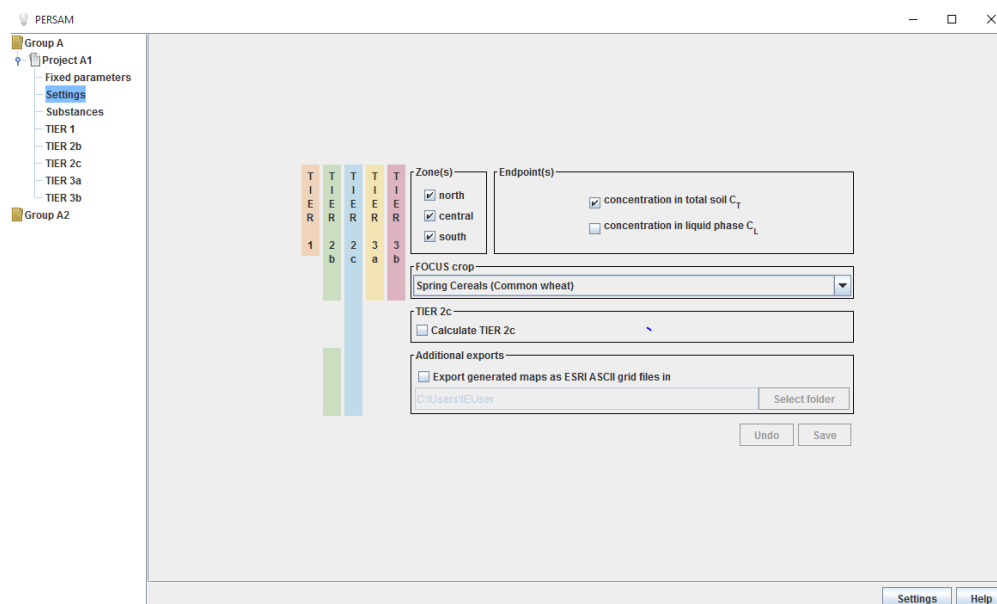
Figure 6: Settings section

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. Click 'Save'

7. Define the Time between applications

8. Click on the 'Input' button for defining the application rate(s) for one or multiple applications. If
    the flag 'Calculate TIER-2C' is selected

    on the settings screen, you have to define also the fraction that reaches the soil (Fsoil).

9. Click 'OK' and 'Save'
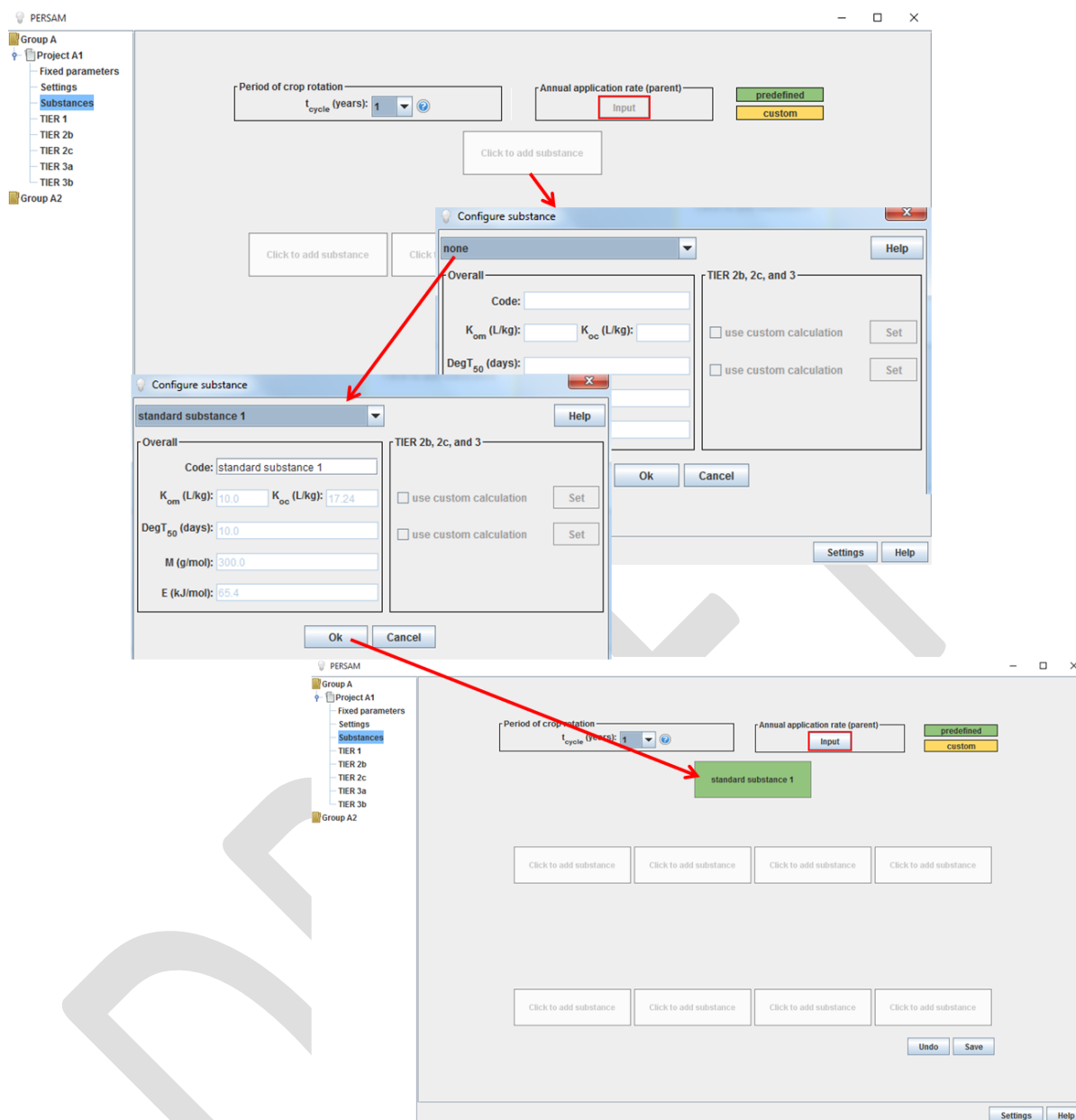
Figure 7: Configure a predefined substance (parent or metabolite)

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

- o Define customized substances or metabolites: see *Configure custom substance*
- o 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
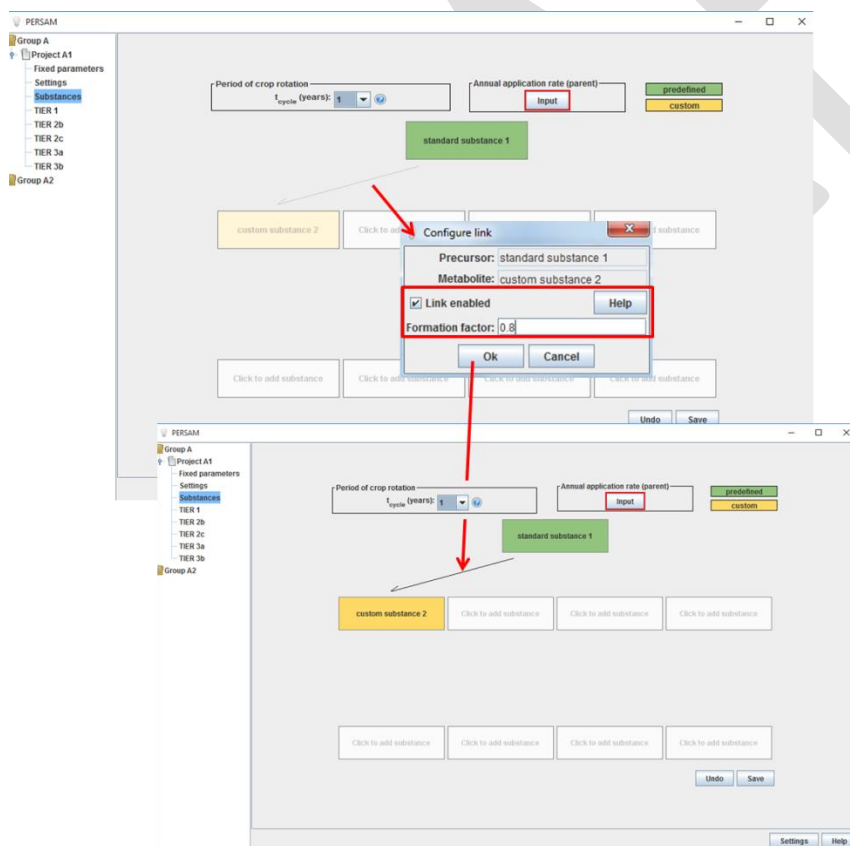
4. Click 'OK'

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.
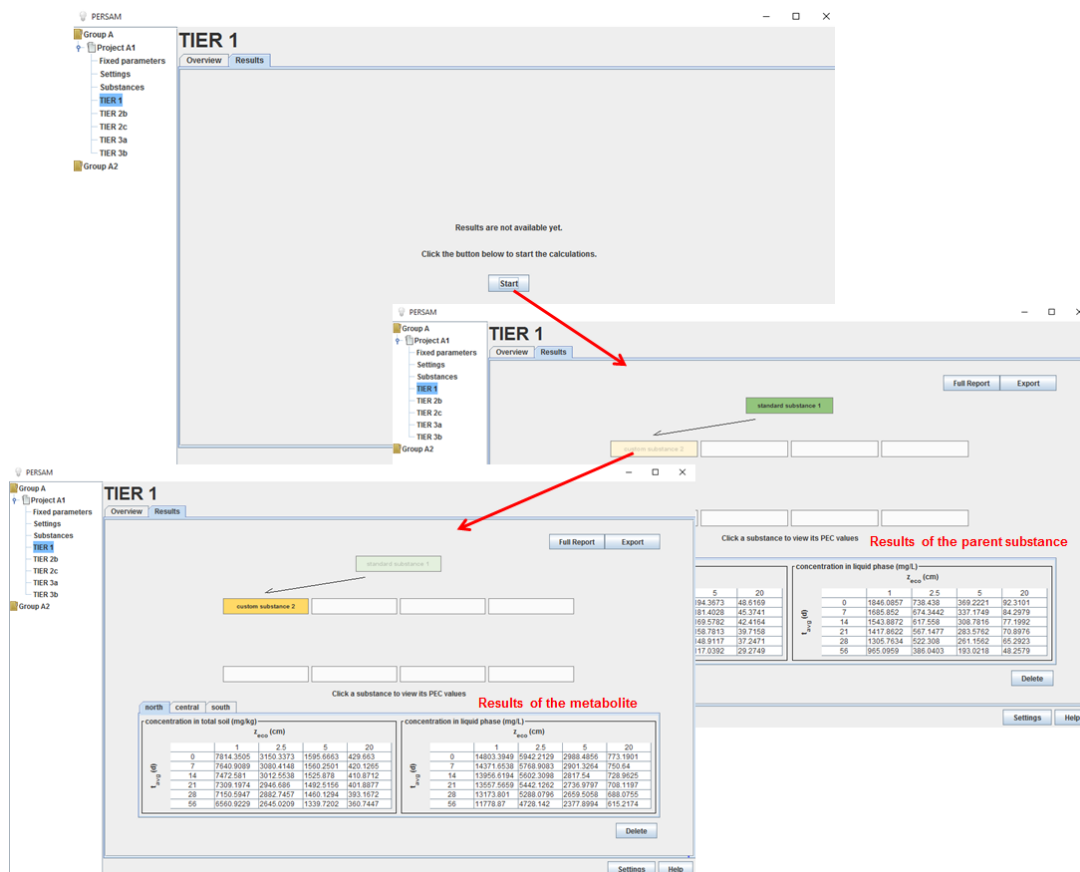
Figure 9: Results of TIER-1

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 95th spatial percentile of calculated PECs for the regulatory selected zone with the related cumulative distribution graph and map.
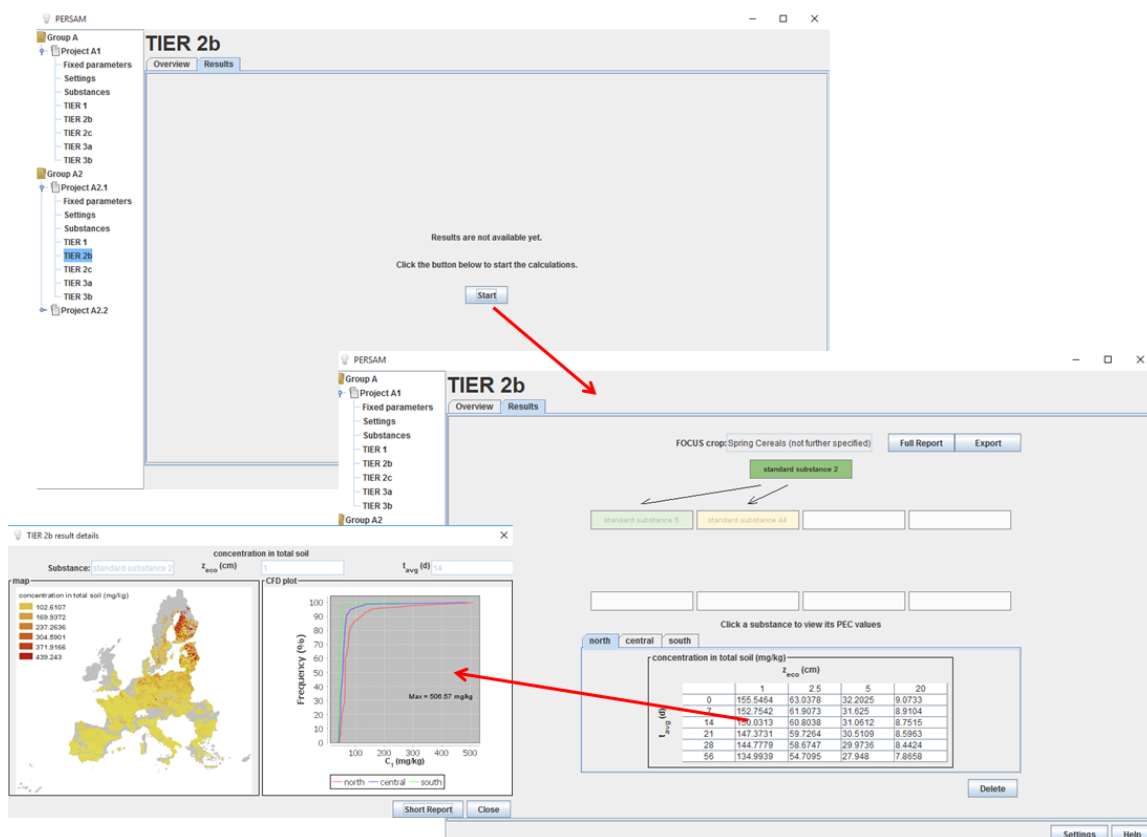
Figure 10:   Results of TIER-2B

How can you perform the TIER-2C calculations?

1. Go to the project tree and select 'Settings'

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 95th spatial percentile of calculated PECs for the regulatory selected zone with the related cumulative distribution graph and map.

How can you perform the TIER-3A calculations?

1. Go to the project tree and select 'TIER-3A'

2. Go to the 'Results' tab

3. Select a substance in the Substance tree to view the results.
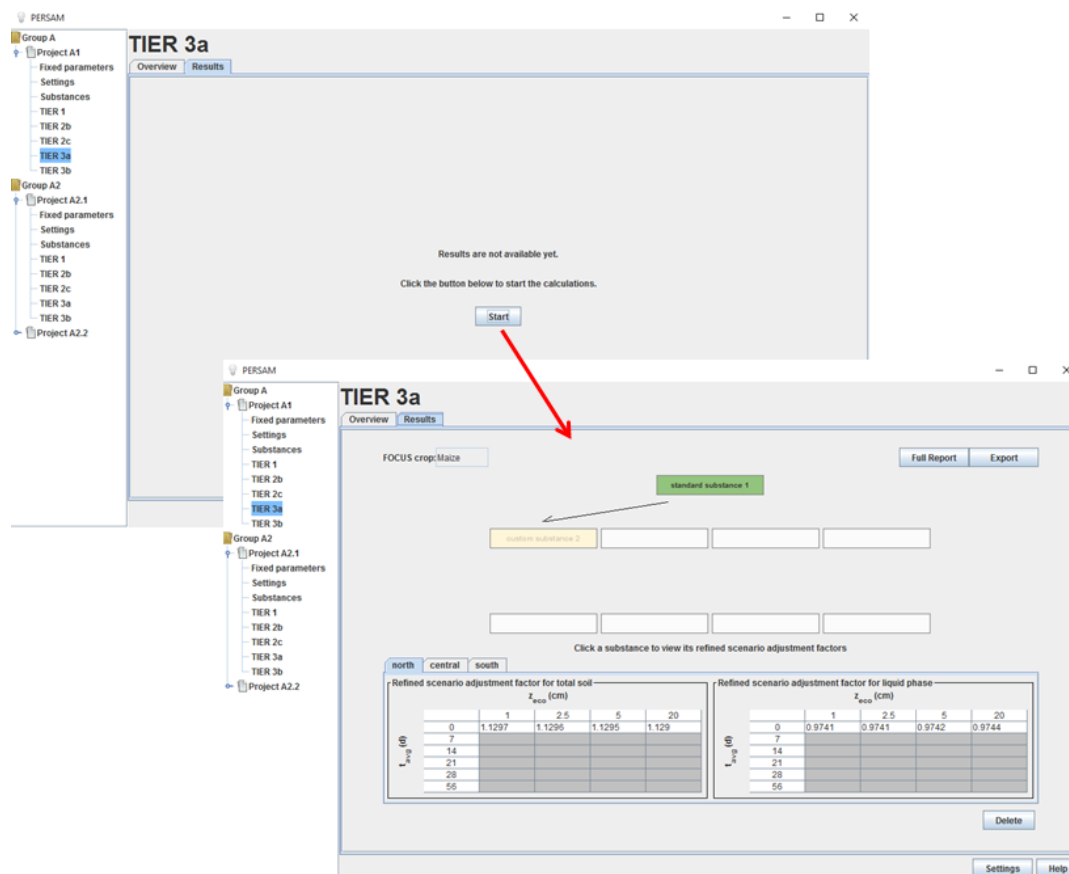
Figure 11:   Results of TIER-3A

How can you perform the TIER-3 B 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.
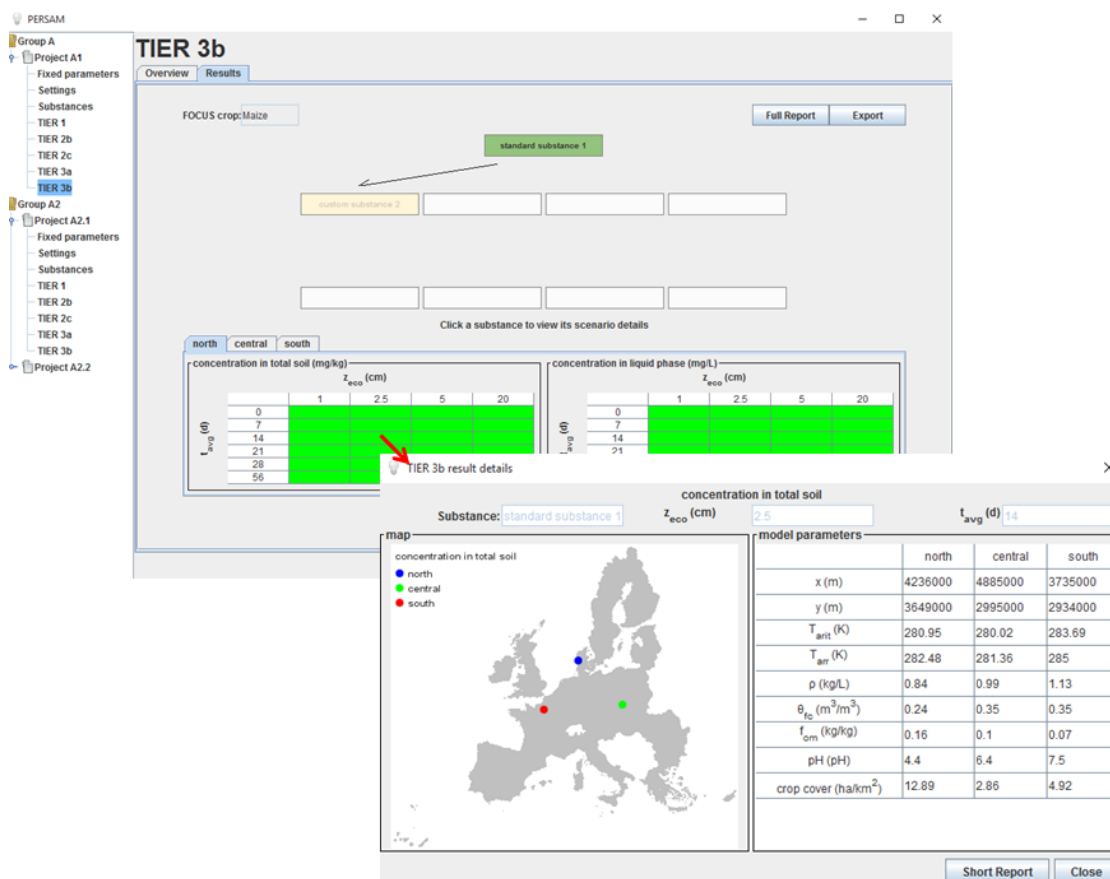
Figure 12:   Results of TIER-3B

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.

- There is an option for automatically generation of pdf reports.

- A copy/paste functionality is not provided in the multiple application rate window. If you want to use the same application rates in another project, copy the project and change afterwards the other properties

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.

Recommendations before starting the installation

- Install the PERSAM software with the user rights of the user who will use the PERSAM tool

- The default installation folder is the 'user' folder. It is important to use a folder where the user has write rights and the folder size can increase to 1 GB.

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:
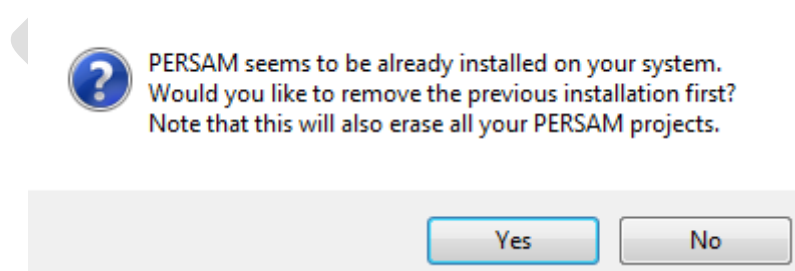
Figure 13: Message 'PERSAM already installed'

   → 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
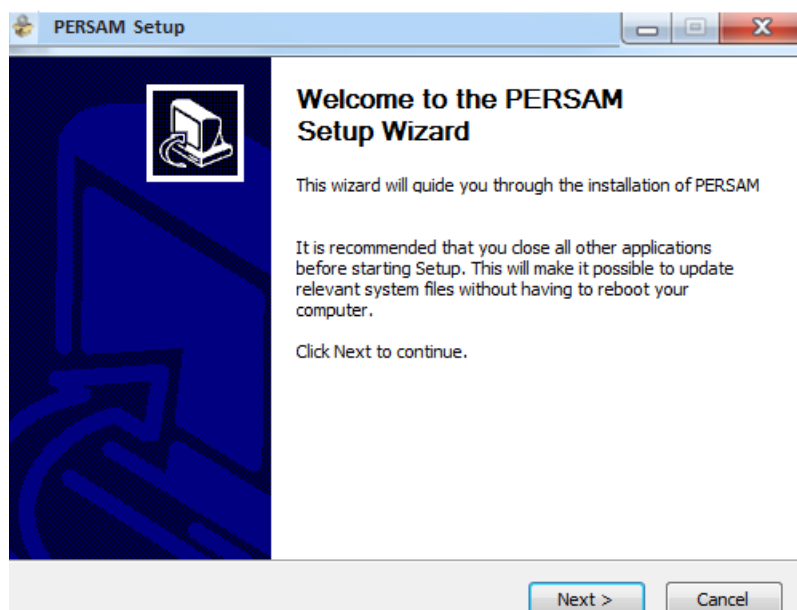
Figure 14:   Installation procedure – Welcome screen

→ Click on 'Next'

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

→ Choose the installation directory:
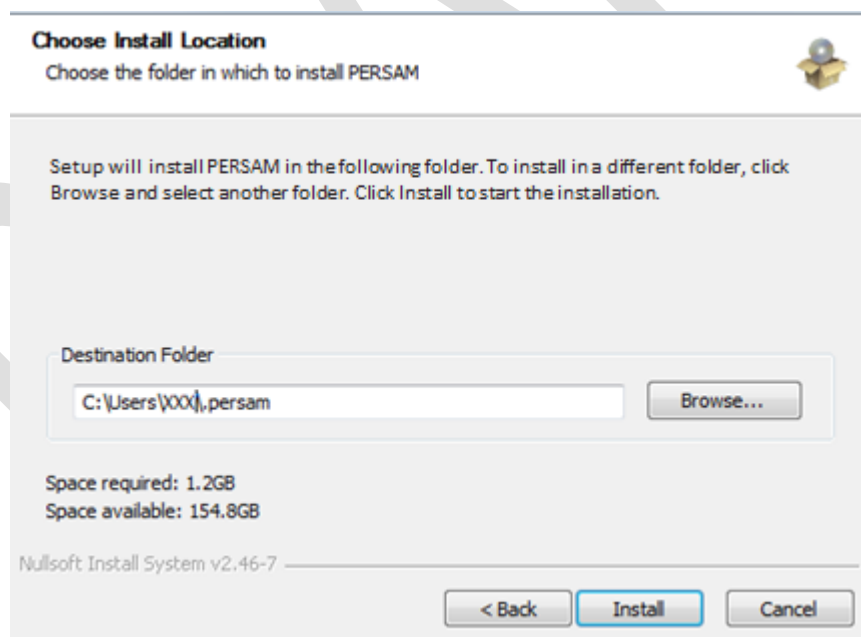
Figure 15:   Installation procedure – Choose installation directory

→ Select the destination folder and click on 'Install'

→ The installation will start
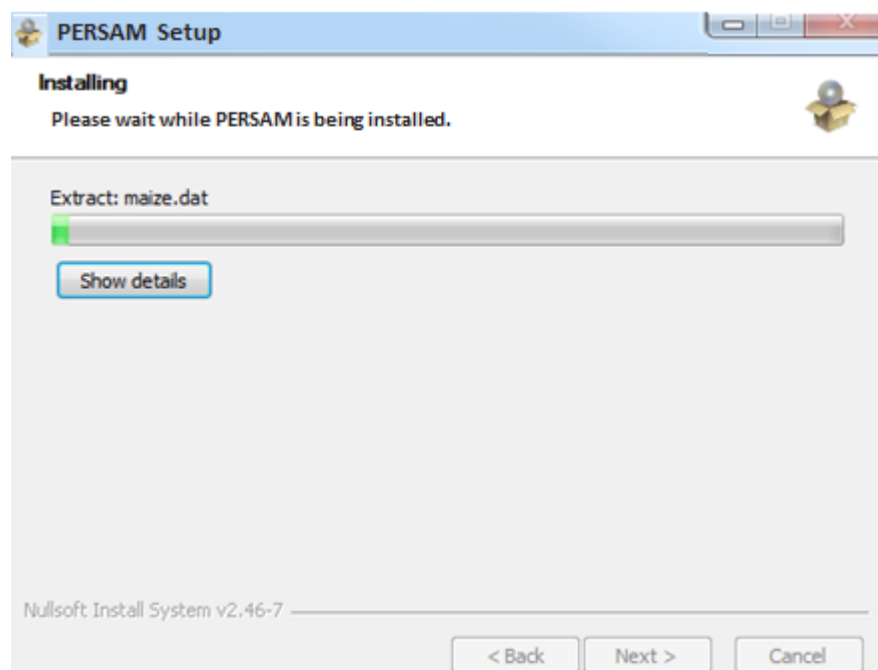
Figure 16:   Installation procedure – Installing the software

→ After the installation, click on 'Finish'

5. You can find the PERSAM application in the start menu of your computer:
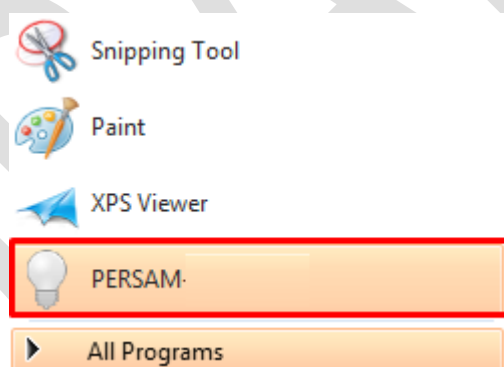
Figure 17:   PERSAM application in start menu

## 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 includes an embedded Java version 1.7.0_80 and 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.

Current PERSAM version number (incl revision number): v2.0.0-Beta1

Figure 18:	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 19:   Project management tree

4.1.   Group

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

Related functionalities:

- o   New group
- o   Rename group
- o   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 20:   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'
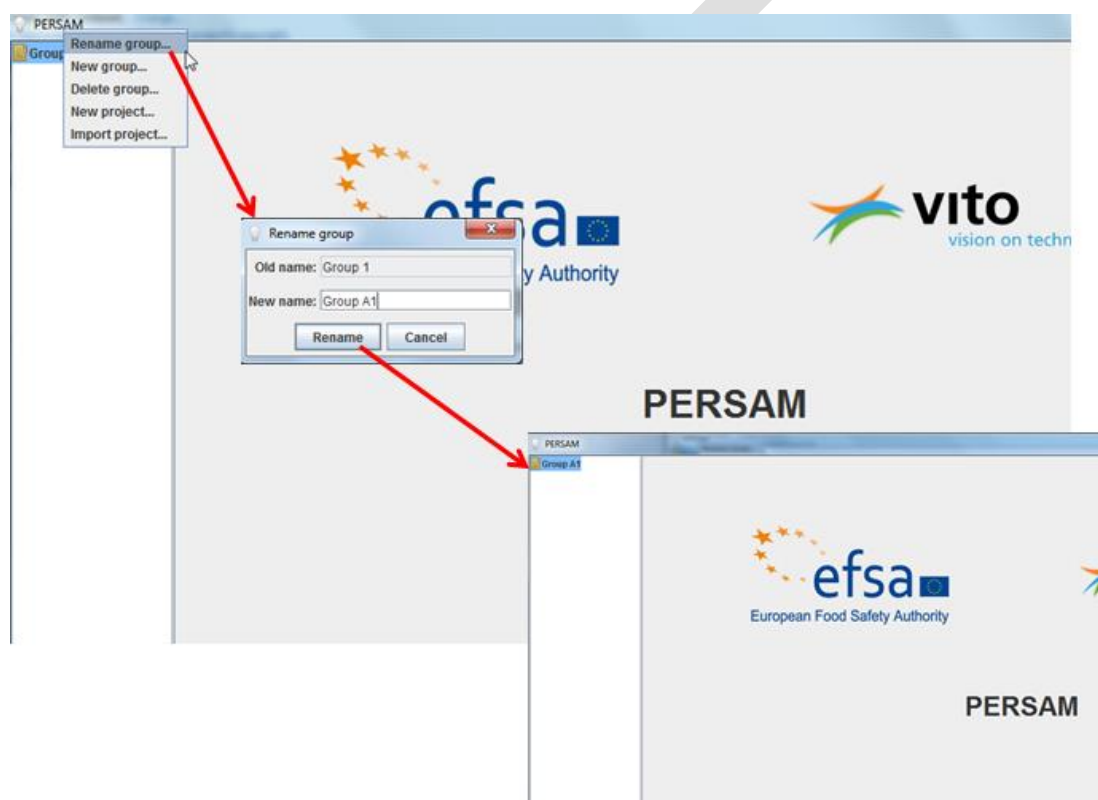
Figure 21:   Rename group

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
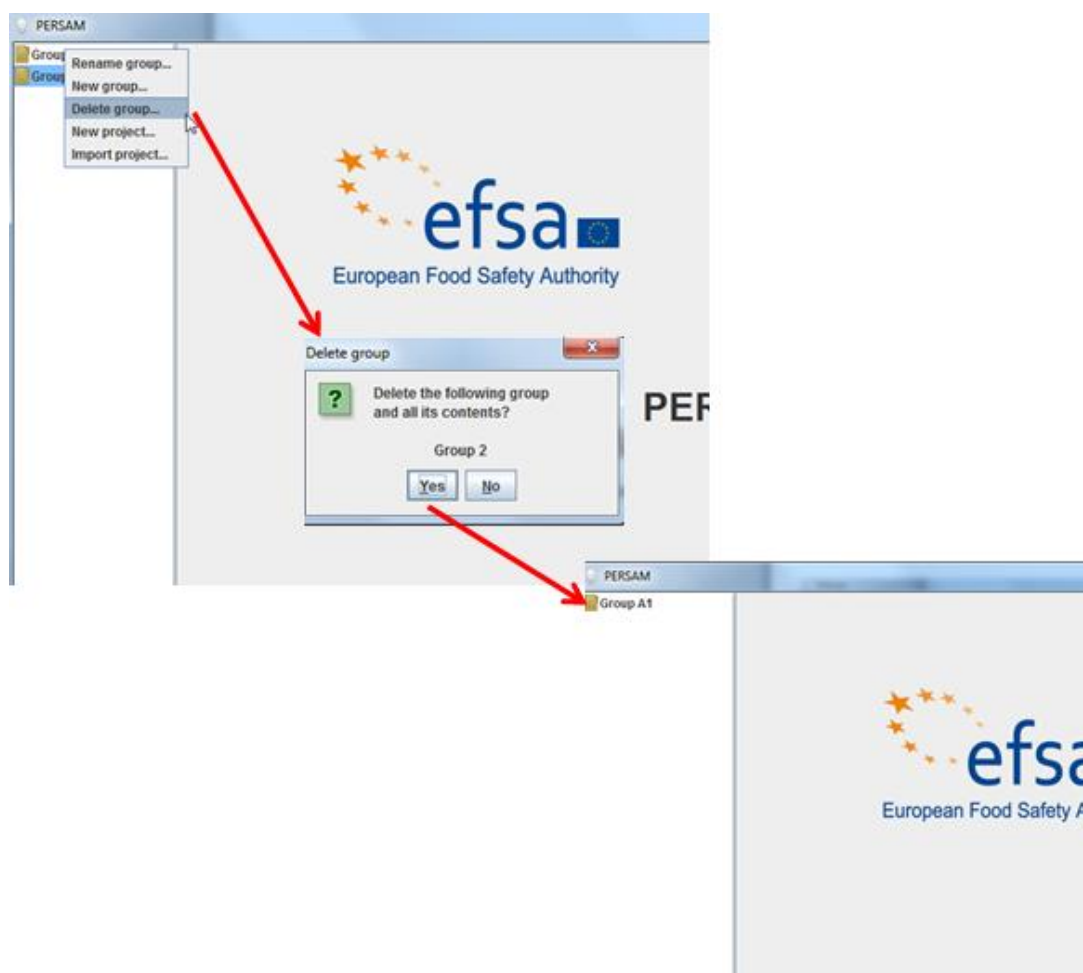
Figure 22:　　Project management – Delete a group

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, TIER-3A and TIER-3B.
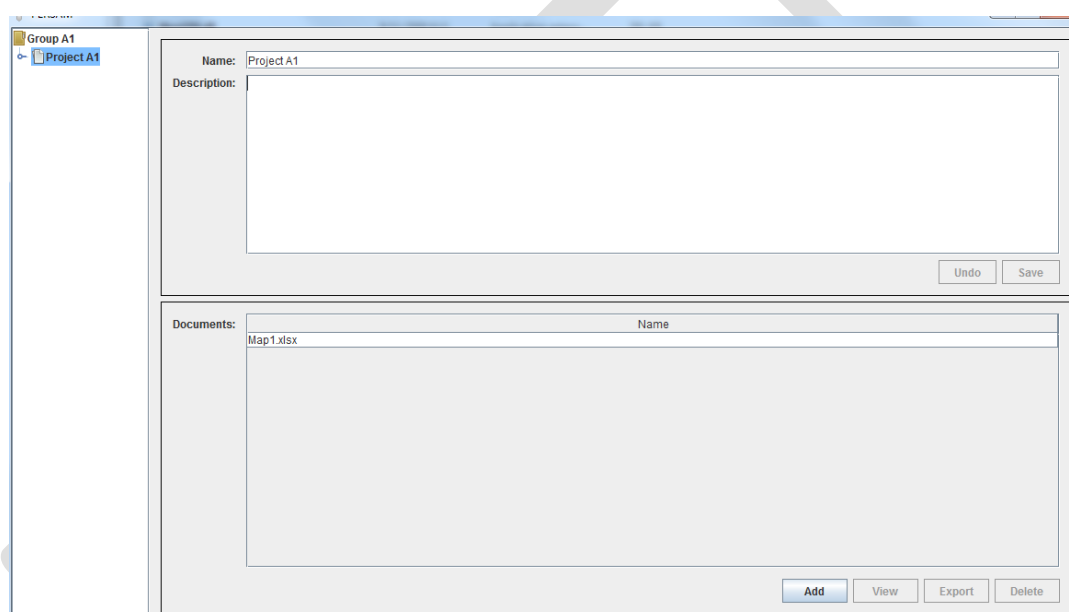
Figure 23:   Project main screen

Documents

The user can add relevant documents to the project.

Other document related functionalities are view, export and delete a document.

Related project functionalities:

- o [New project](#)
- o [Rename project](#)
- o [Copy/Paste project](#)
- o [Delete project](#)
- o [Import project](#)
- o [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'
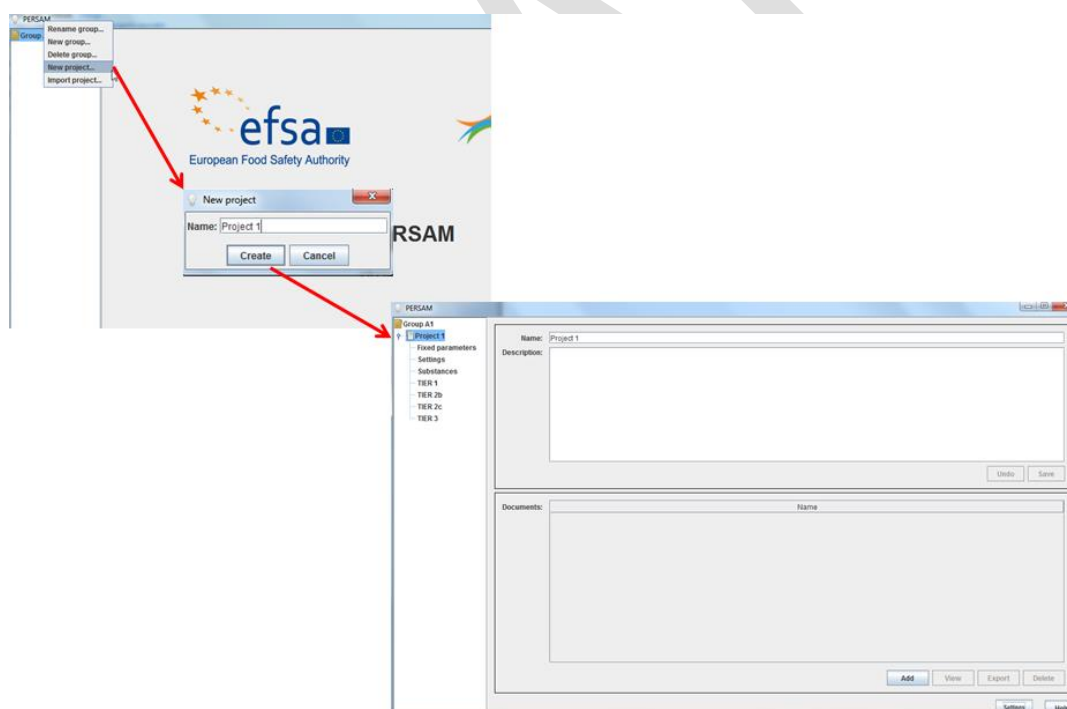
Figure 24:   New project

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'
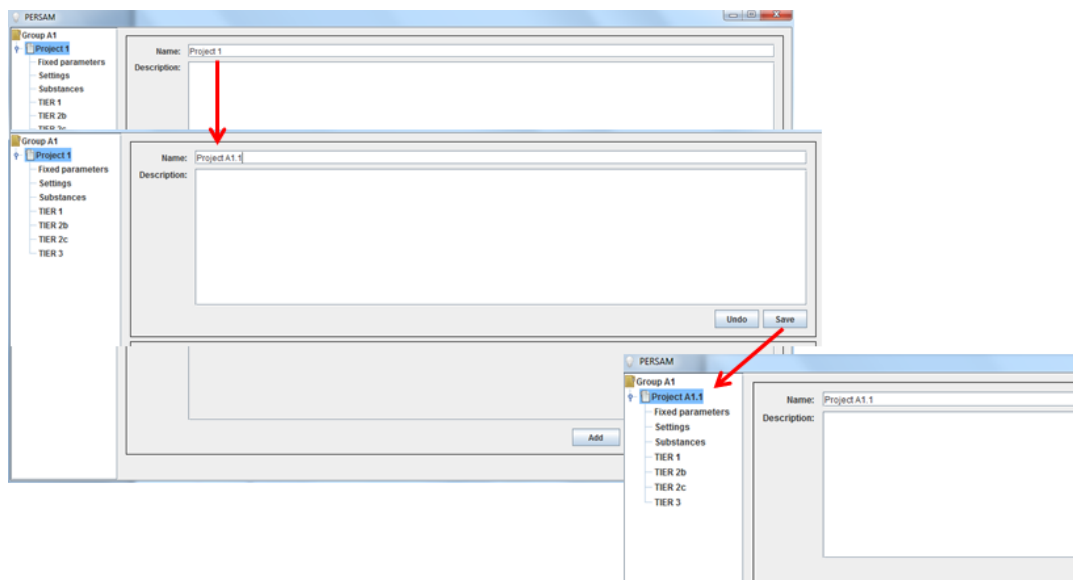
Figure 25:   Rename project

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.
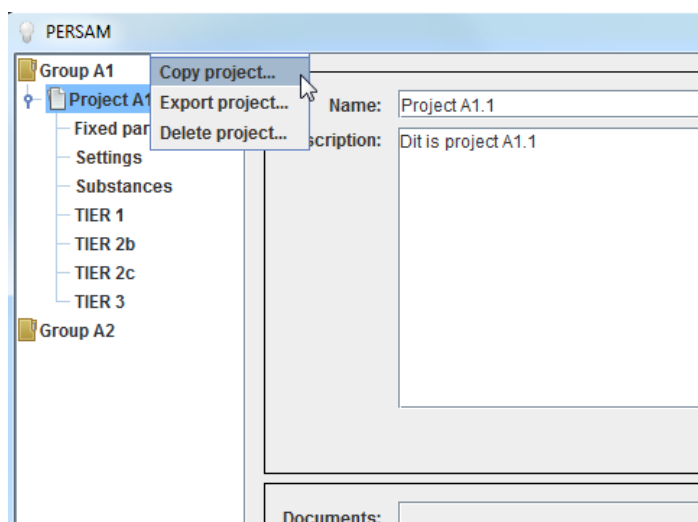
Figure 26:   Project management – Copy project

3. Select the group where you want to place the copied project

4. Right click and select 'Paste project'
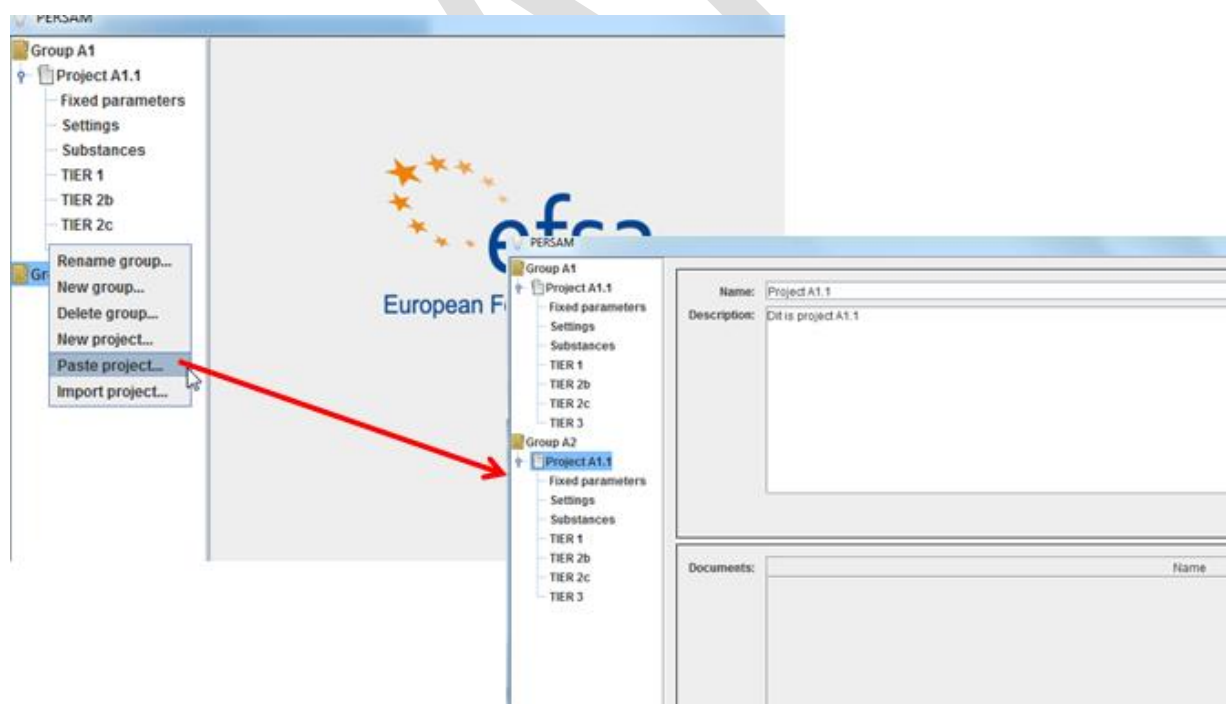
Figure 27:   Project management – Past project

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
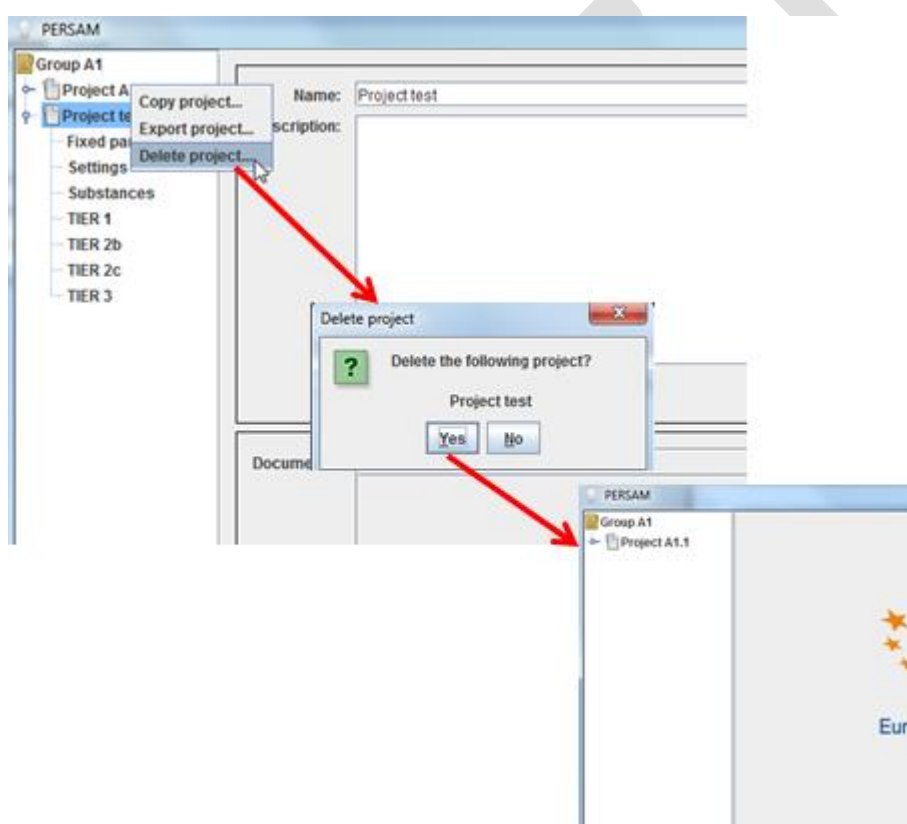
**Figure 28:**   Project management – Delete project

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.

**Note:** _If you import a project from a previous version of PERSAM, the current version of PERSAM takes the first FOCUS crop of the_ FOCUS crop list _where PERSAM crop corresponds with CAPRI crop from the imported project._
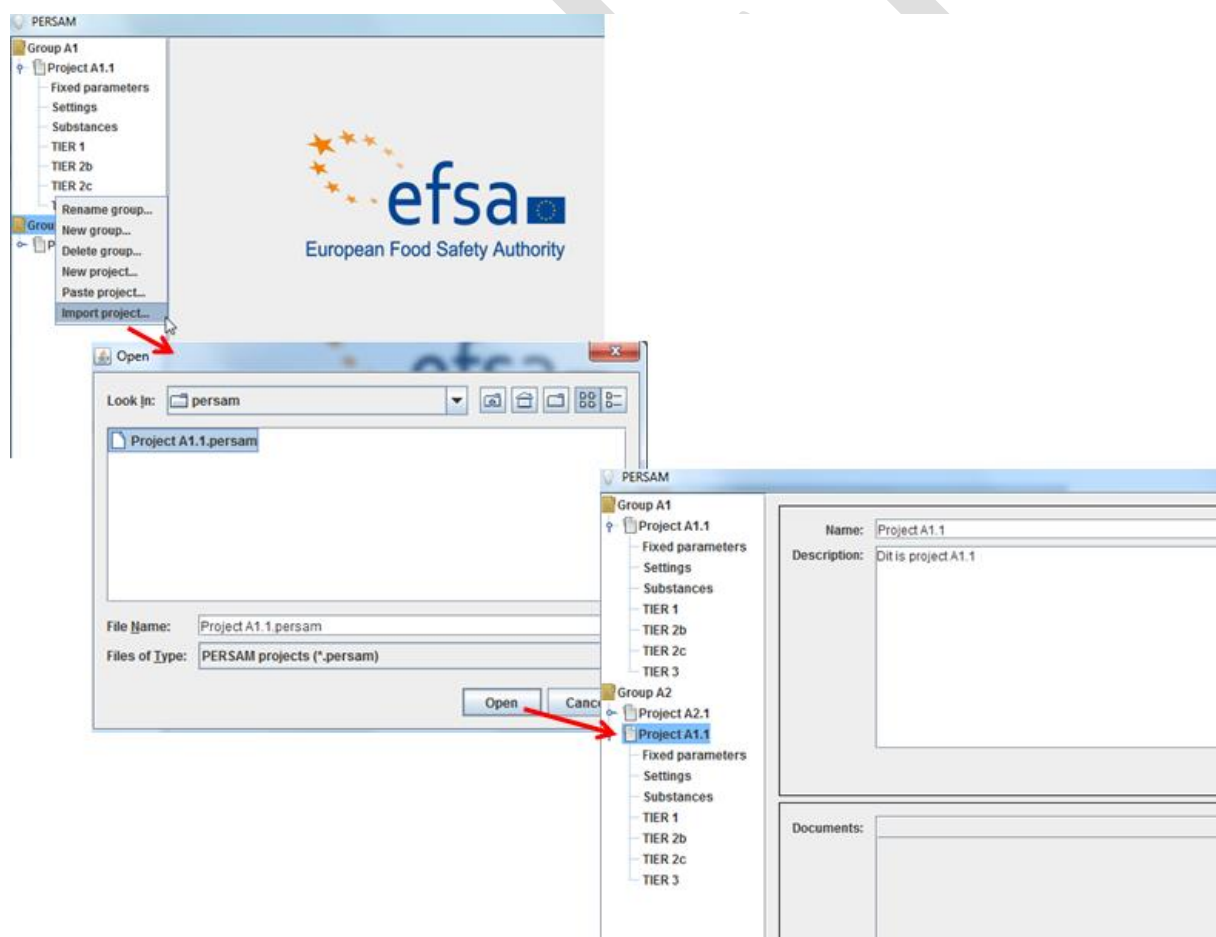
Figure 29:   Project management – Import project

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.
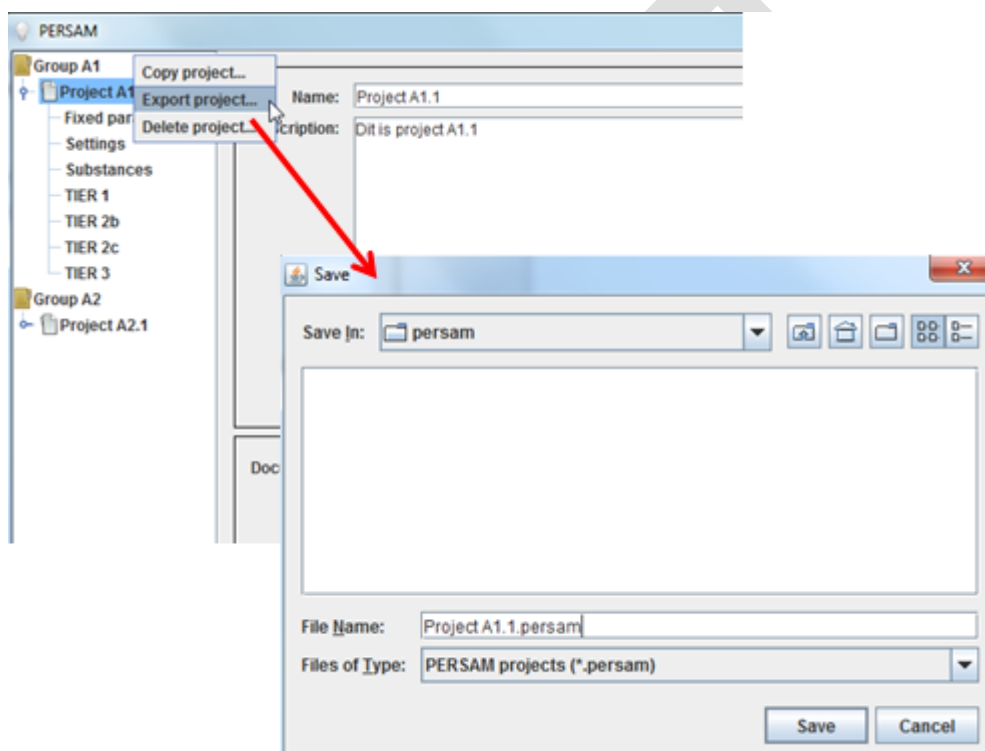
Figure 30: Project management – Export project

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:

- o   Excel
- o   Word
- o   PDF
- o   TXT
- o   CSV

Document management
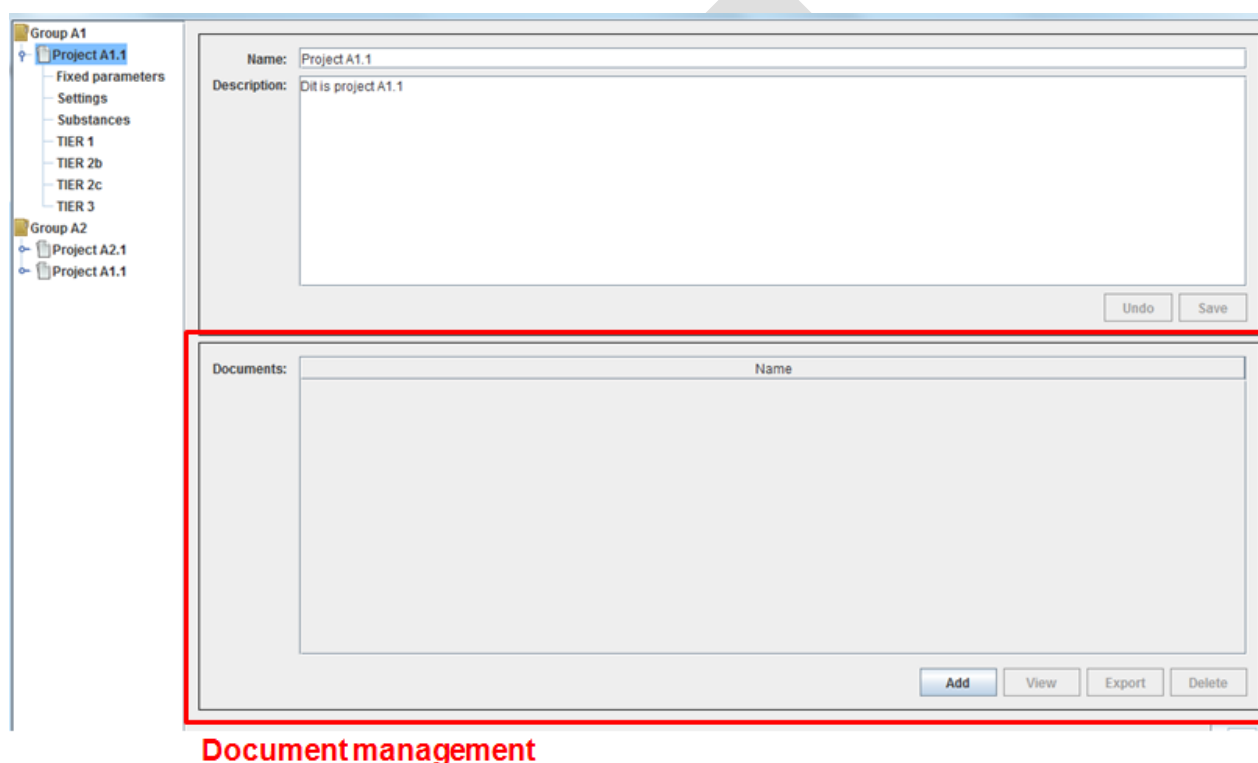
Figure 31:   Project – Document management

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.
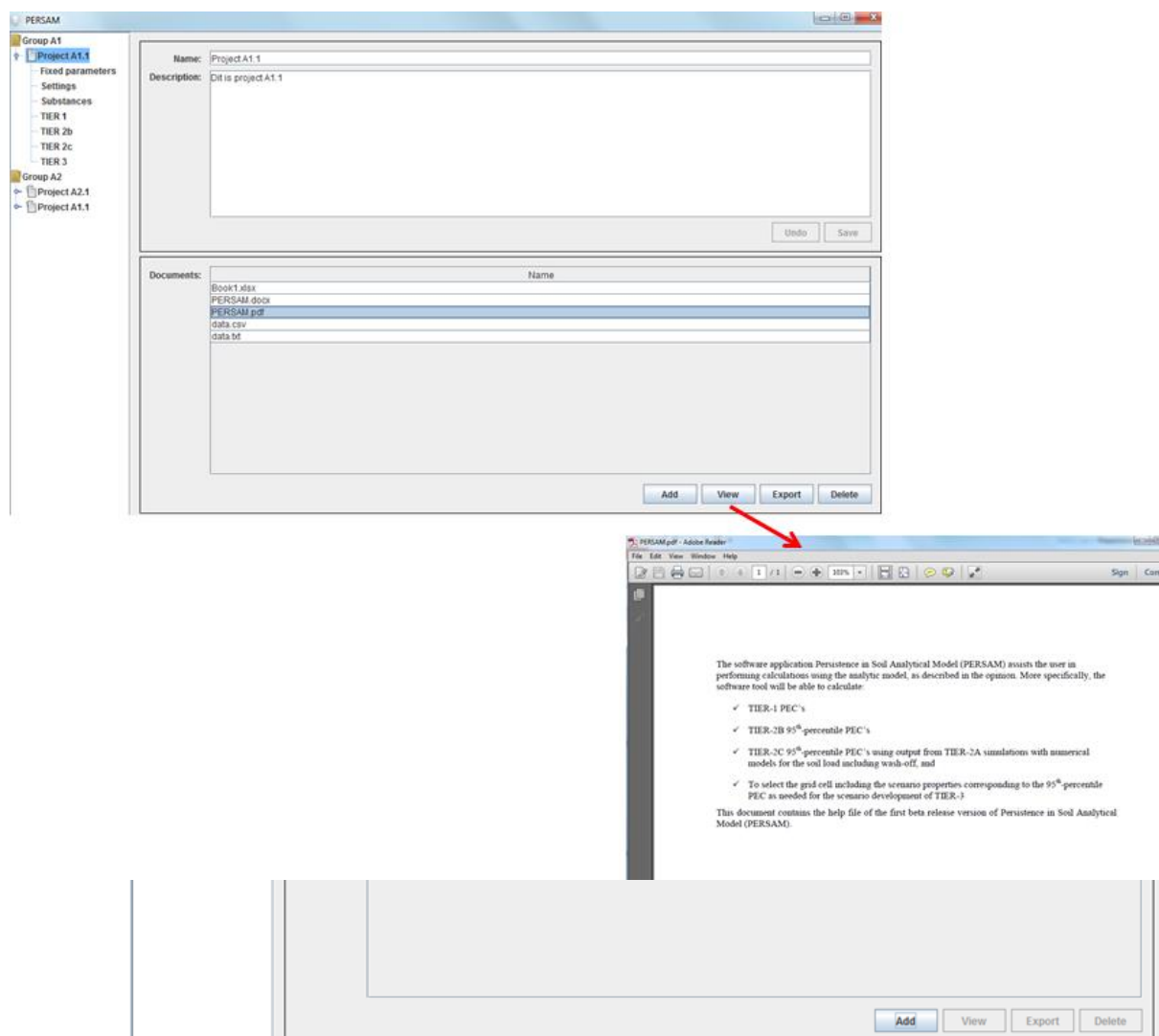
Figure 32:   Document management – Add document

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 33:   Document management – View document

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'
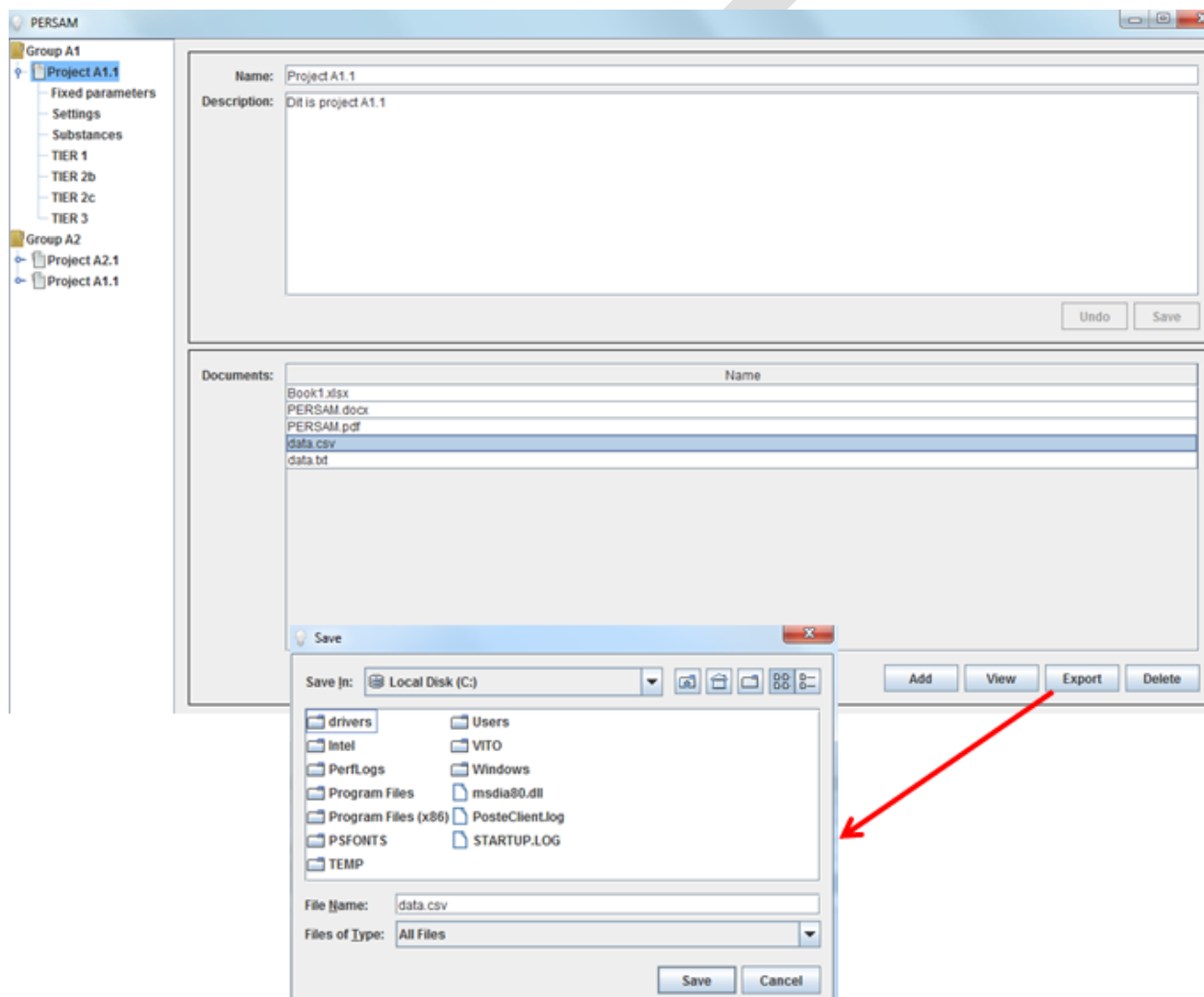
Figure 34: Document management – Export document

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
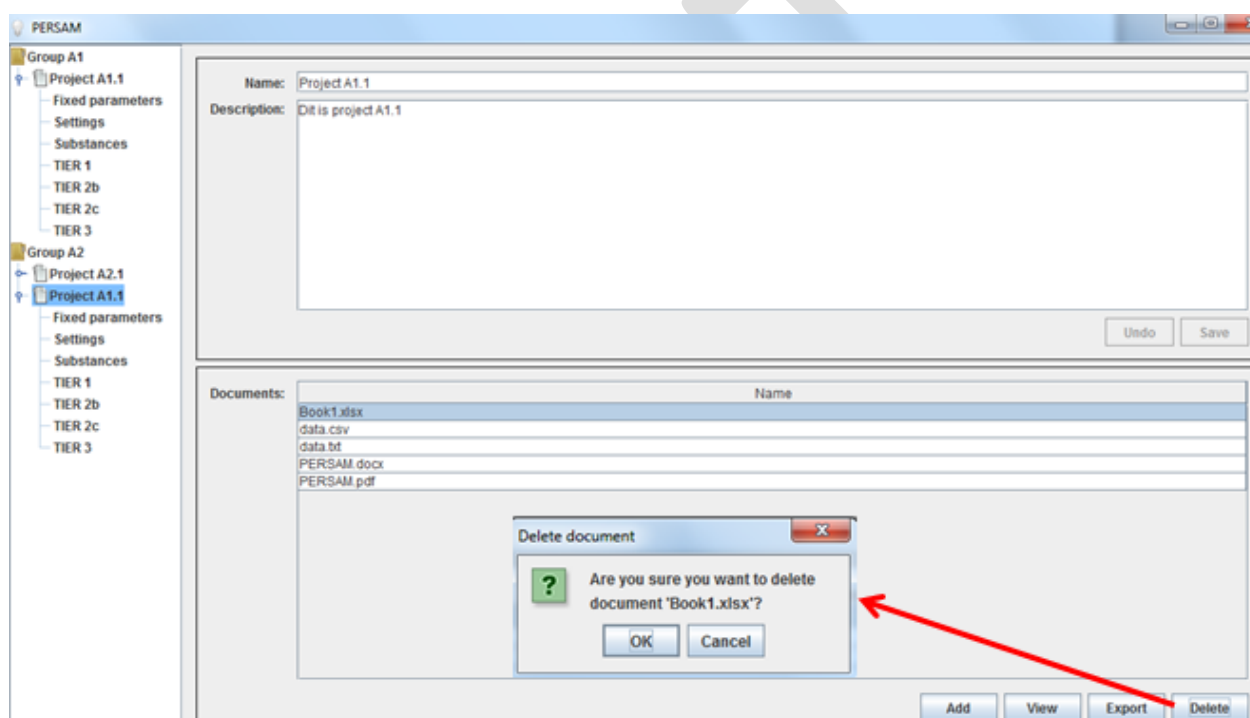
Figure 35:   Document management – Delete document

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

Parameter	Symbol	Unit	Default values
Ecotoxicological averaging depth	z_{eco}	cm	1; 2.5; 5; 20
Plough depth	z_{til}	cm	20
Gas constant	R	kJ.mol^{-1}.K^{-}	0.008314
Reference temperature	T_{ref}	K	293.15
Time period since application over	t_{avg}	days	0; 7; 14; 21; 28; 56
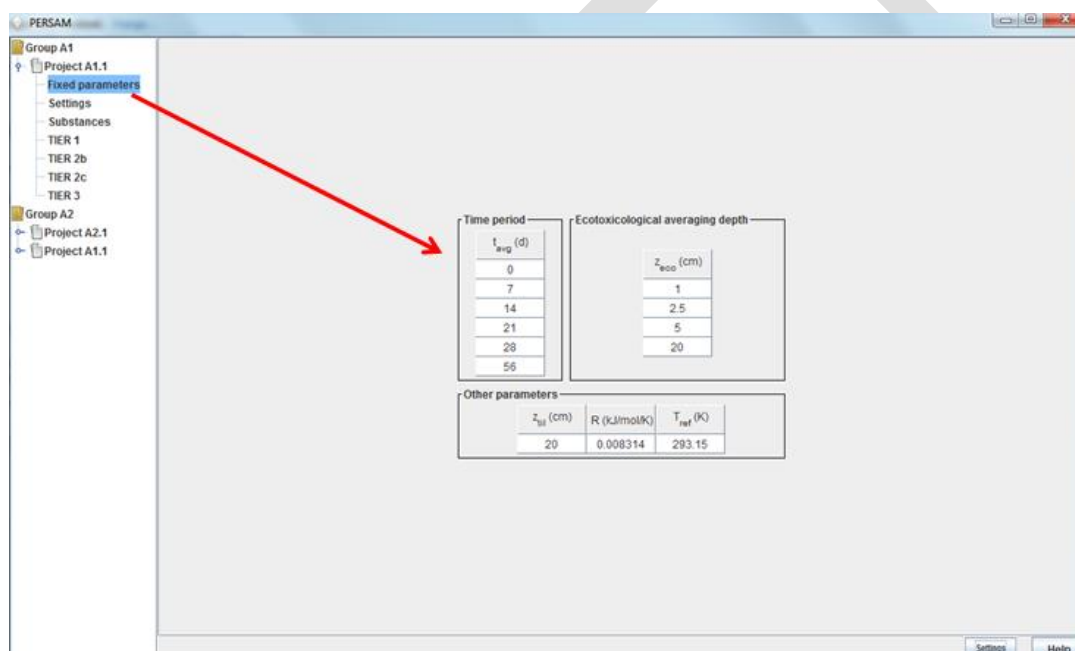
Figure 36:   Fixed parameters

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}) 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 Center South	By default all zones are checked	TIER-1, TIER-2B, TIER-2C, TIER-3A and TIER-3B
Endpoints	Concentration in total soil C_T		TIER-1, TIER-2B, TIER-2C, TIER-3A and TIER-3B
	Concentration in liquid phase C_L		
Focus Crop		see FOCUS crop list	TIER-1, TIER-2B, TIER-2C, TIER-3A and TIER-3B
Calculate TIER-2C			TIER-2C
Additional exports	Exported generated maps	By default this parameter is not selected	TIER-1, TIER-2B, TIER-2C, TIER-3A and TIER-3B

When the checkbox in the 'Additional exports' section is enabled, the tool will export all generated maps in TIERs 2b, 2c, 3a and 3b 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.
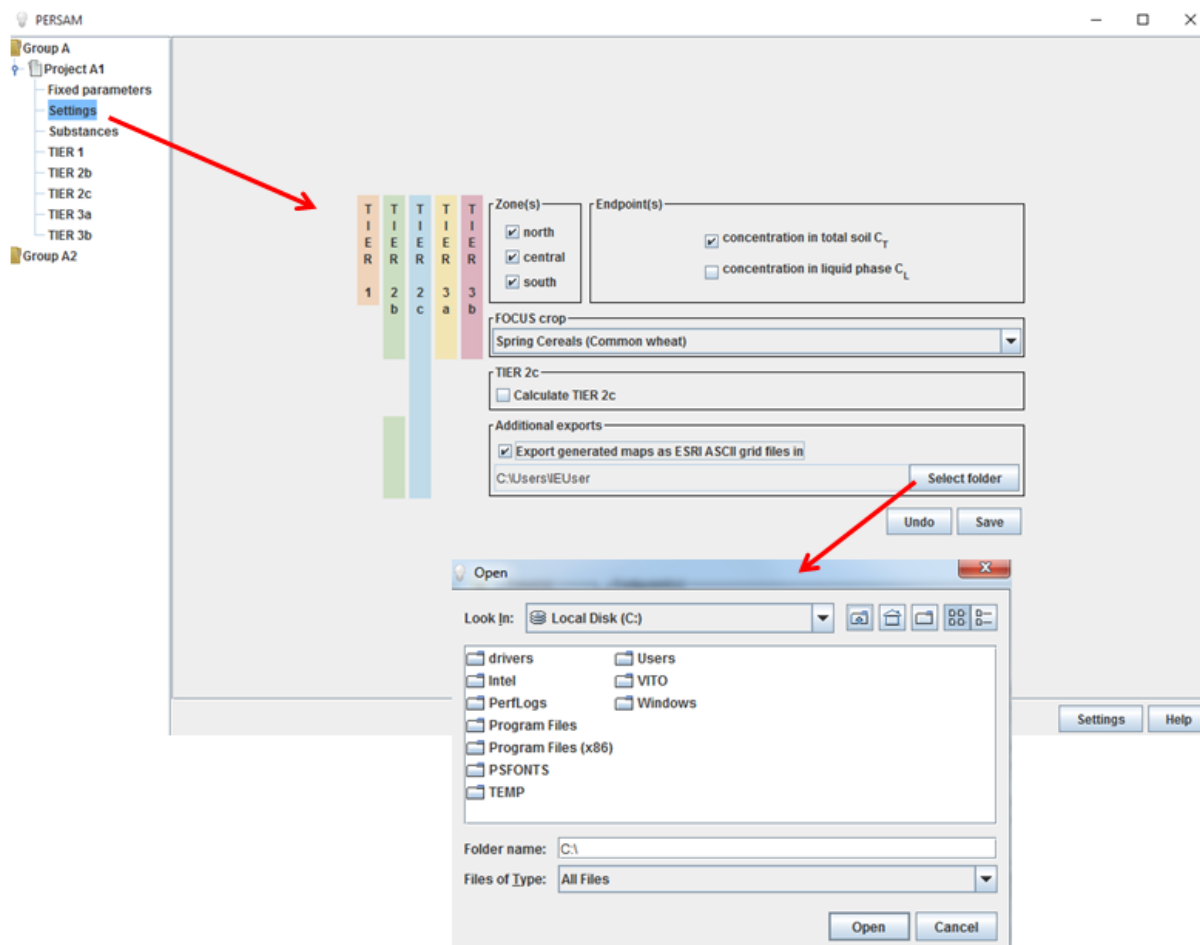
Figure 37:   Settings section

If changes have been made, and the user navigates away from the screen without clicking the save button, the following warning pops up.
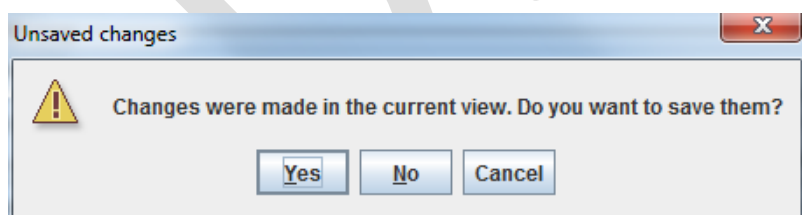
Figure 38:   Dialog Unsaved changes

- 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.
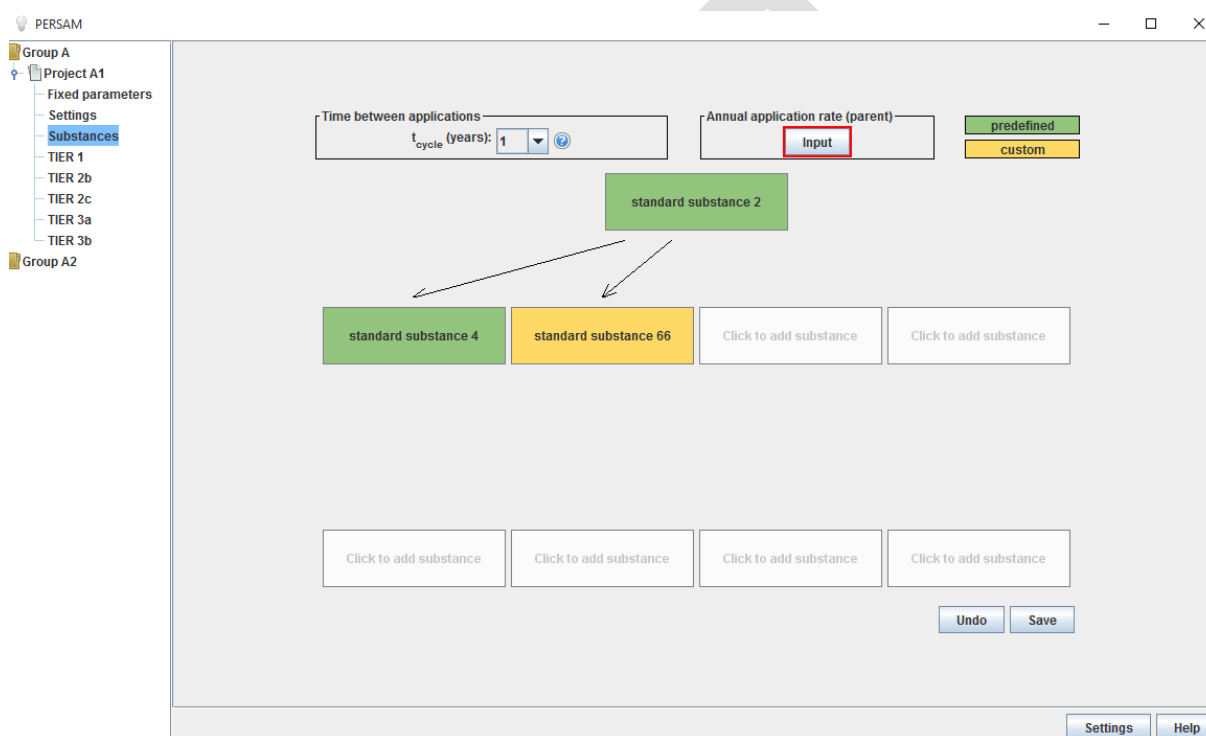
Figure 39:   Substances section

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	DegT50	days	
Organic matter/water	K_{om}	l/kg	
Organic carbon/water	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:

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

7.1.   Configure Application rate(s)

The user defines the application rate(s) and the fraction that reaches the soil (fsoil) for one or more applications.

1. Define first the substance tree and click on 'Save'.
   Remark: The 'Input' button is by default disabled because you need to define first the substance tree.

2. Click on the 'Input' button and the multiple applications window appears.
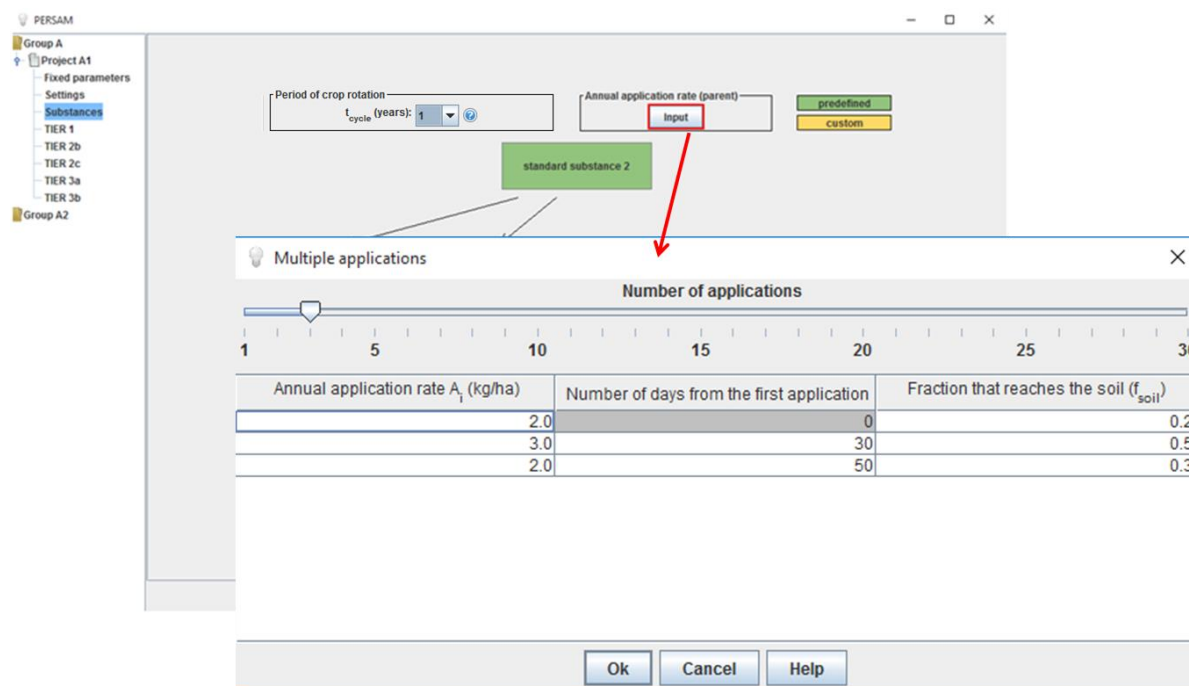
Figure 40:   Multiple applications – Define application rate(s) & f_{soil}

3. Define the annual application rate for the first application. The default value for the number of days from the first application is 0 and cannot be changed.

4. If the check box 'Calculate TIER 2c' is checked in the settings screen, it is obligated to define the Fraction that reaches the soil (fsoil).

    If the check box 'Calculate TIER 2c' is not checked in the settings screen, fsoil is disabled.

    Remark: *0 ≤ the value of fsoil ≤ 1*

5. If you want to define the application rate for multiple applications, use the slider for adding new rows to the table.

    The number of days must be between 0 and 365.

    Define always the application rates according the number of days in ascending order.

    Remark: *the number of days from the first application of the previous row < the number of days from the first application of the current row*

    the number of days from the first application of the current row < the number of days from the first application of the next row

6. Click 'OK'

PERSAM calculations based on the input of the multiple applications window:

1) Calculate **residues in soil** with:

$$Rp_i \quad = \quad A_{i-1} * exp \left(-[\ ln(2)/DegT50]\ * t_i \right) \qquad\qquad (1)$$

Rp_i: residues i remaining from previous applications $i\text{-}1$ (g/ha) (Rp_1 is set to 0)
A_i: total actual application rate of app. no. i (g/ha)
$DegT50$:   half life of the substance at scenario temperature (d)
t_i: time since the last application for application no i (d)

2) The **current rate of application A_i** is calculated based on the nominal application rate, the fraction reaching the soil and residues remaining from previous applications:

$$A_i \quad = \quad NA_i * f_{soil,i} \quad + Rp_i \qquad\qquad (2)$$

NA_i: nominal application rate no. i in the sequence of applications (g/ha)
$f_{soil,i}$:   fraction of application i reaching the soil (-)
Rp_i: residues remaining from previous applications considered for application no i (g/ha)

3) The **calculation in PERSAM** is done using as application rate the maximum calculated A_i. $f_{soil,I}$ is not further used in the PERSAM calculation as it is already taken into account in the calculation of A_i. PERSAM users must be able to give for each application A_i, $f_{soil,I}$, t_i.

<u>Tip:</u> A copy/paste functionality is not provided in the multiple application rate window. If you want to use the same application rates in another project, copy the project and change afterwards the other properties.

7.2.   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.
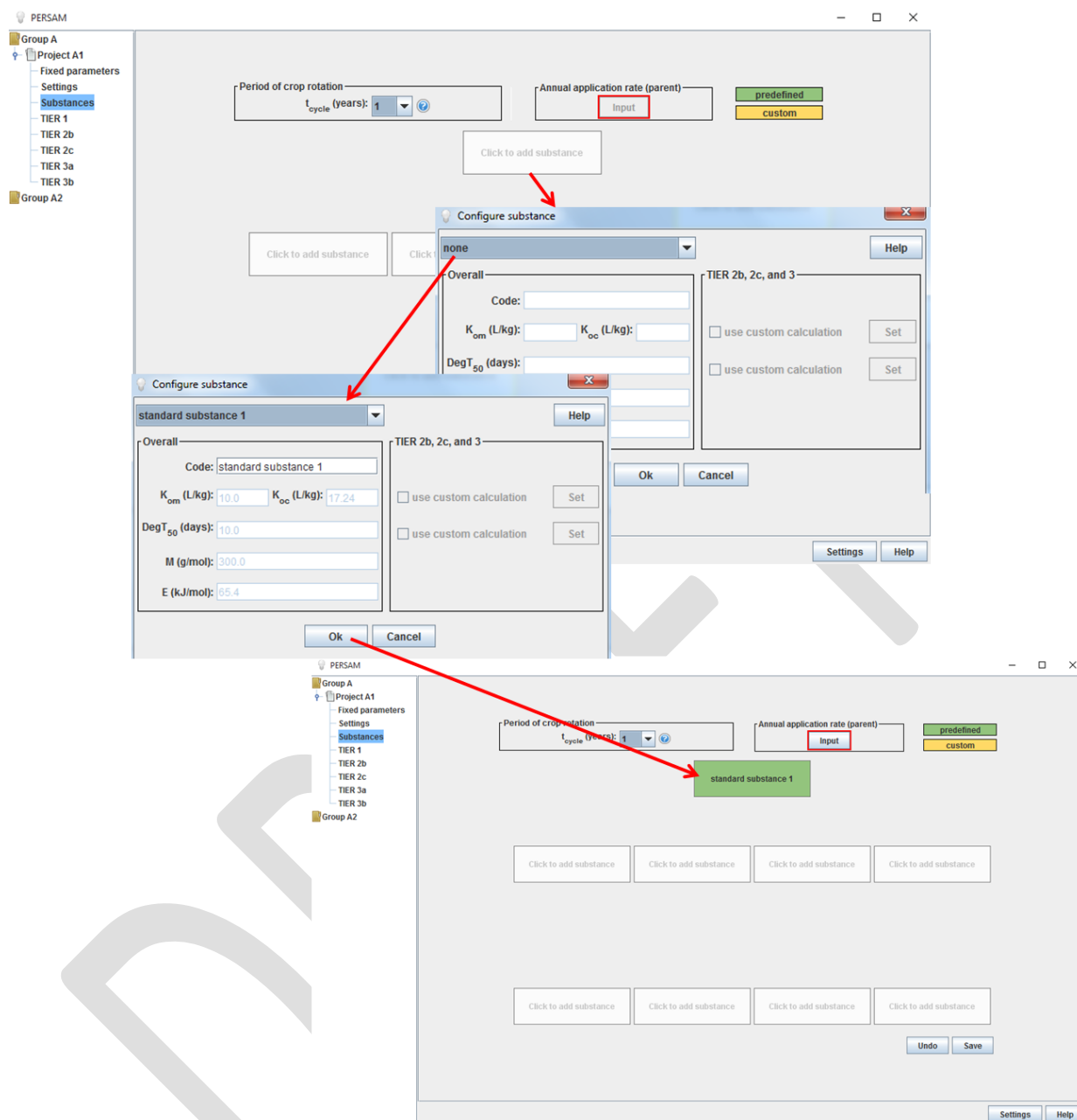
Figure 41:   Configure a predefined substance (parent or metabolite)

7.3. 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:
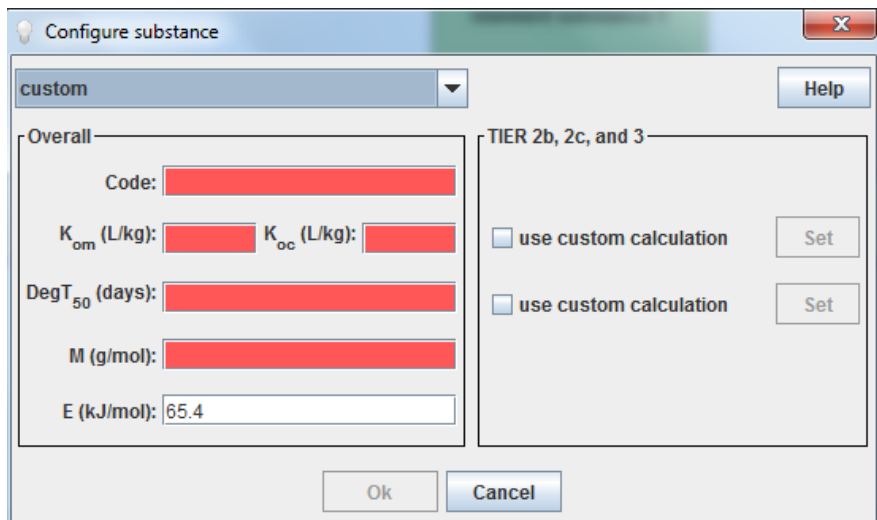
1. Click on a place holder in the tree and the screen 'Configure substance' appears.

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'
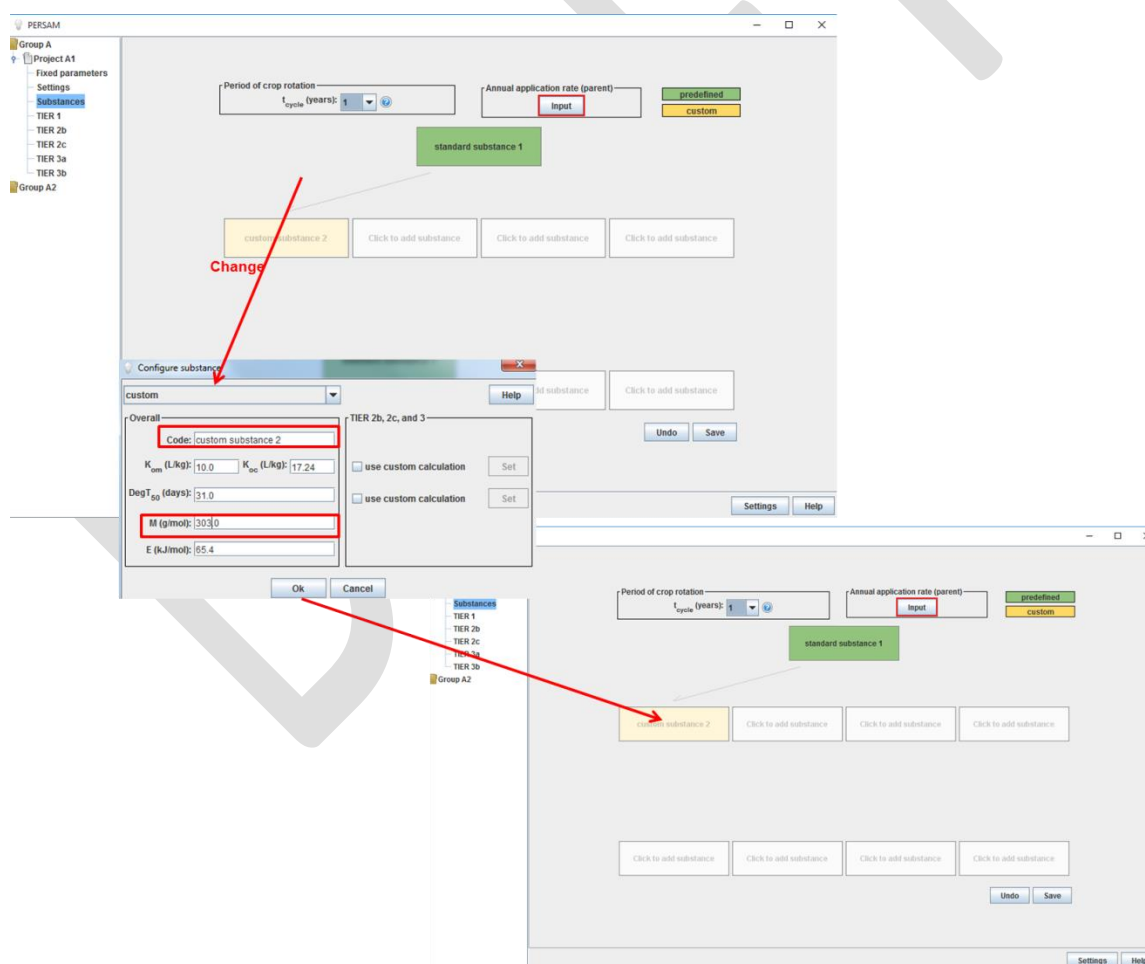
Figure 42:   Configure a customized substance, starting from a predefined substance

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 43:   Configure a new customized substance

4. Click on 'OK'

7.4.   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
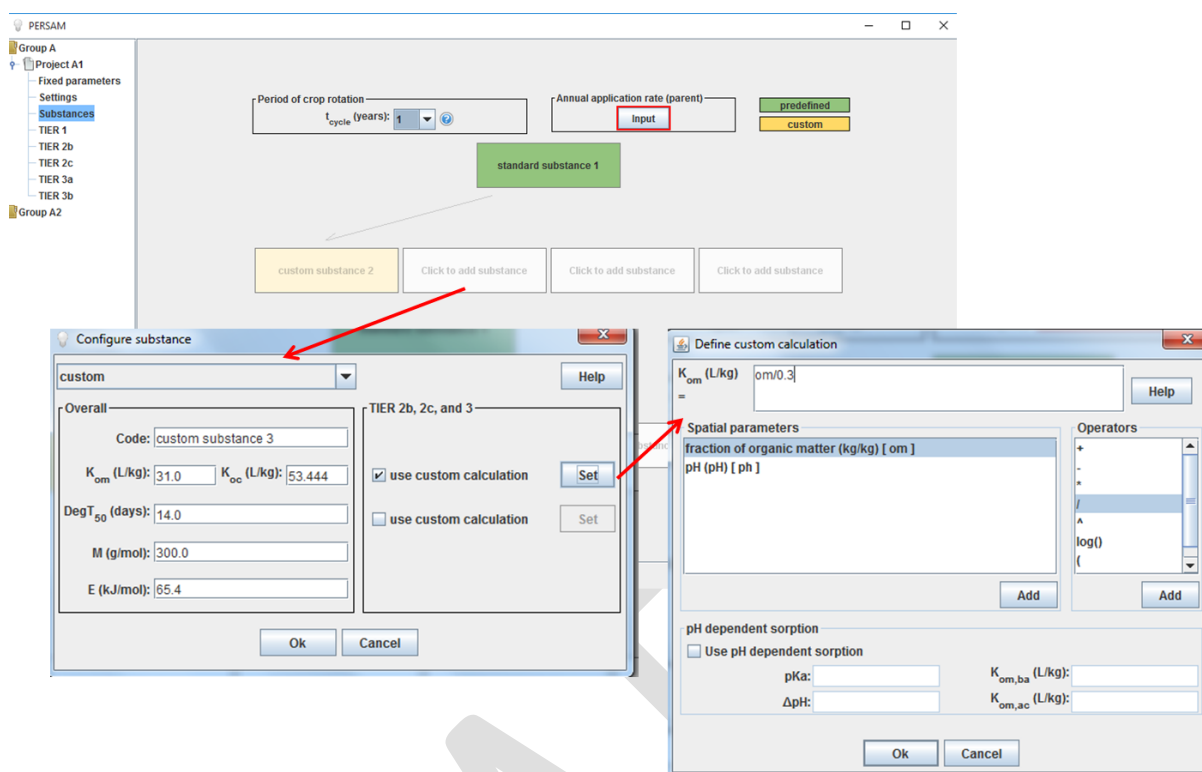
Figure 44:   Define custom calculation for K_{om}

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'.

Formula for pH dependent sorption:

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

pKa: negative logarithm of the dissociation constant

pH: pH correction factor

$K_\mathrm{OM,\ ba}$: organic matter/water distribution coefficient under basic conditions

$K_\mathrm{OM,\ ac}$: organic matter/water distribution coefficient under acid conditions

Limit Kom/DegT50 to user min and max values:

1. Select the checkbox 'Set minimum' and/or 'Set maximum'.
2. Enter the corresponding parameter min and/or max for Kom or DegT50
3. Click 'OK'

Calculation rules based user min/max values for K_om/DegT50:
- Calculated value for K_om/DegT50 < Min value → use Min value
- Calculated value for K_om/DegT50 > Max value → use Max value

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( )

7.5. 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
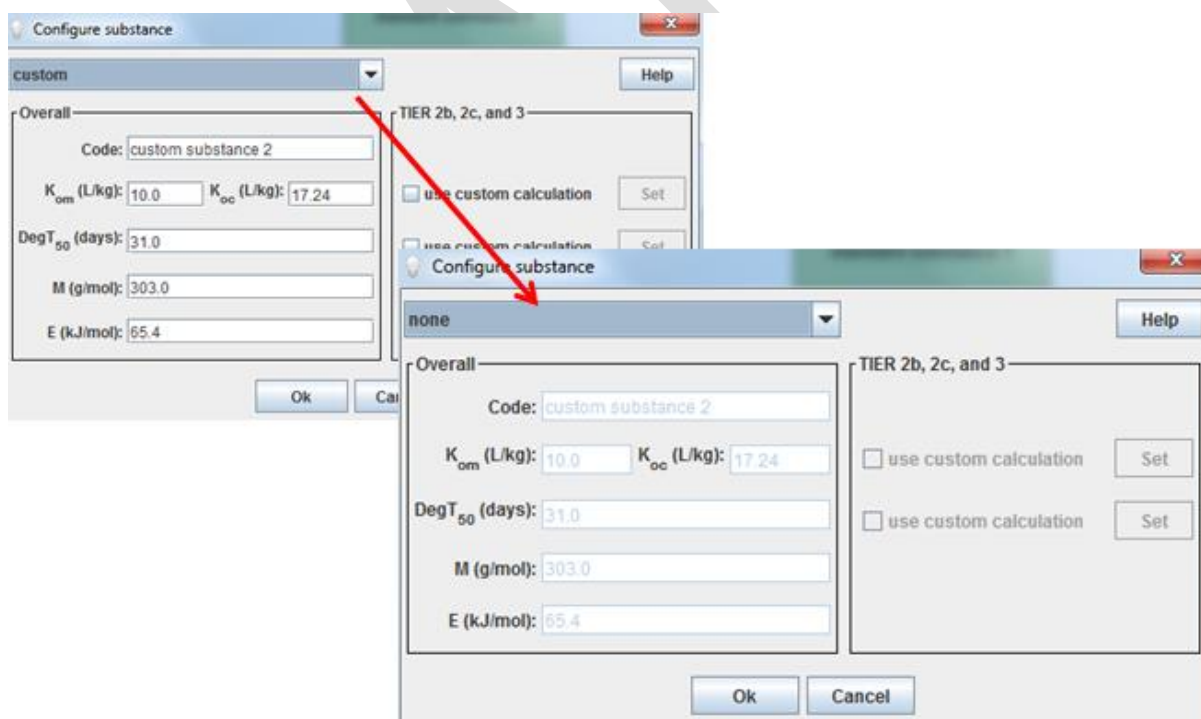
Figure 45: Delete a configured substance

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

7.6.   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'
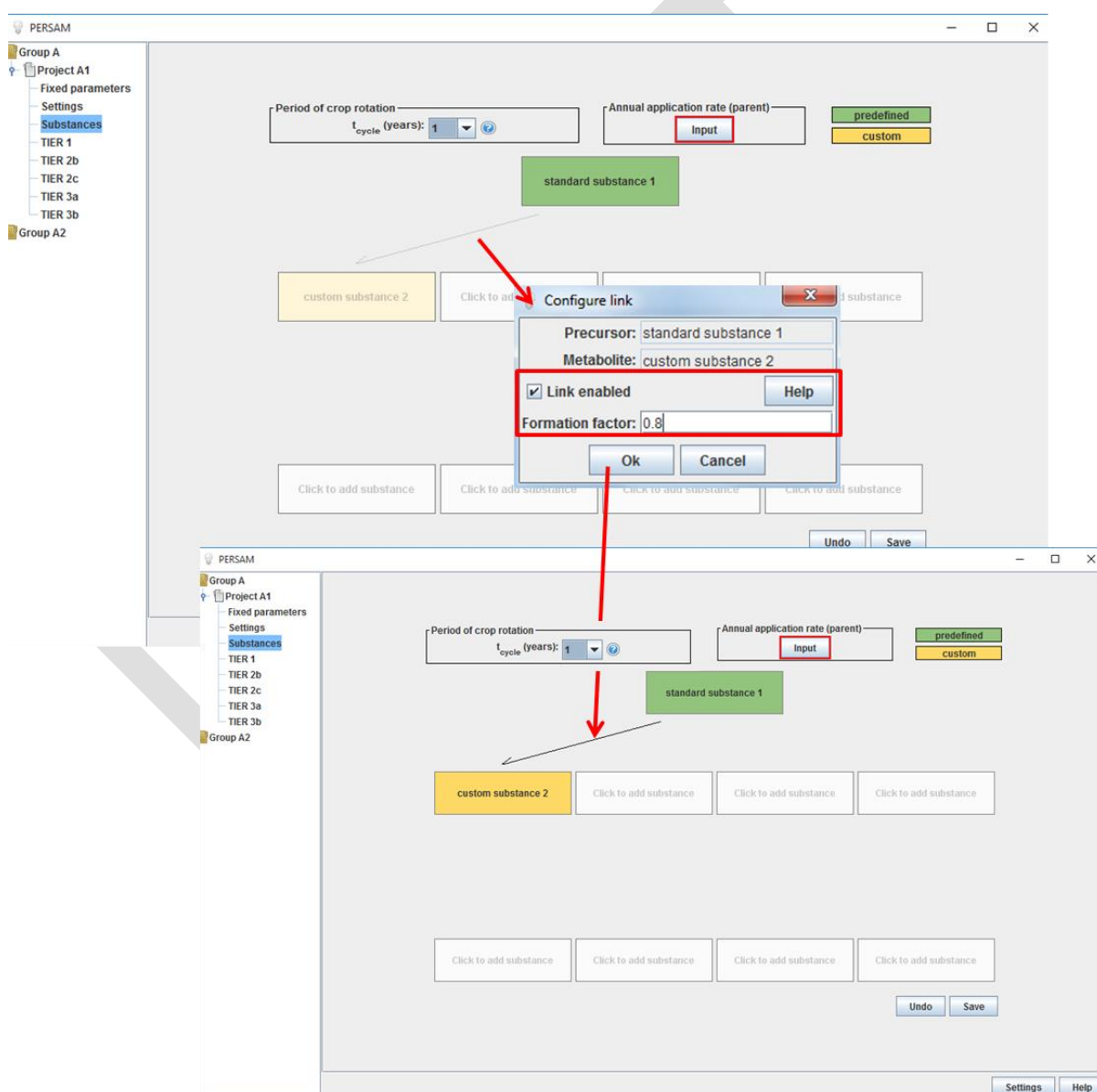
Figure 46:   Configure a link

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.

7.7.   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.
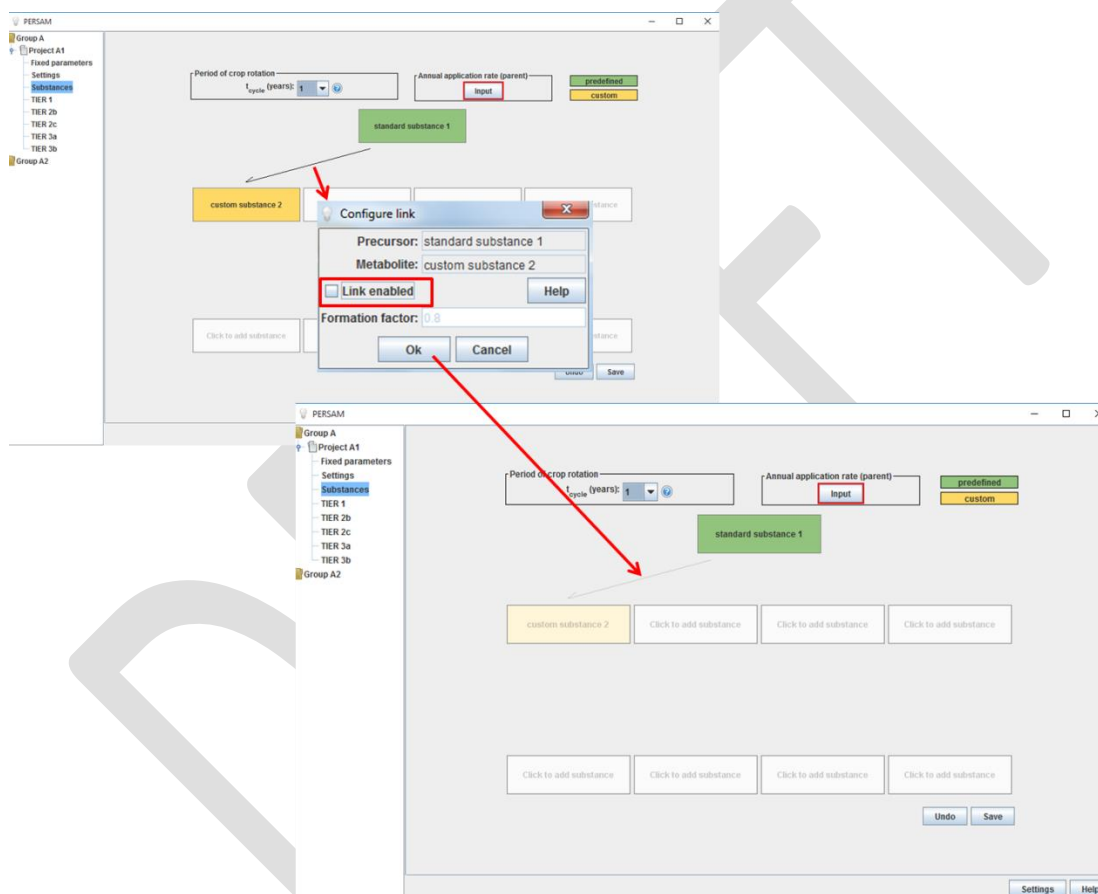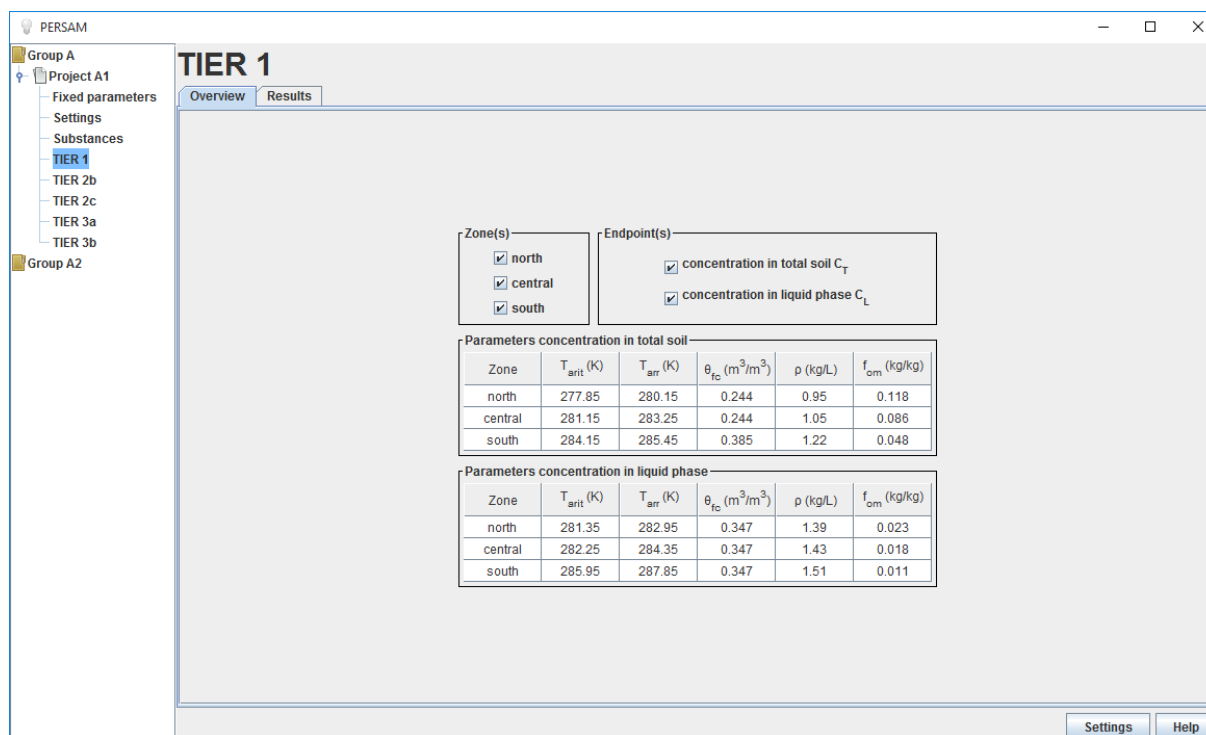
Figure 47:   Delete a link

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 48:   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:

- o   Zone(s) (see settings section)

- o   Endpoint(s) (see settings section)

- o   Substances (parent & metabolites) (see substance section)

8.2.   TIER-1 calculations

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

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^{-1}.K^{-1}	0.008314
Reference temperature	Tref	K	293.15
Arrhenius weighted average soil temperature	T_{arr}	K	Corresponding to parameter T in formula 4
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 $C_{T,peak}$

Parameter	Symbol	Unit	Default values/Input
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 $C_{L,peak}$

Parameter	Symbol	Unit	Default values/Input
Maximum total concentration in soil	$C_{T,peak}$	mg.kg^{-1}	Formula 3
Volumetric water content	θ_{fc}	m^3.m^{-3}	Soil-specific parameter
Dry bulk density	ρ	kg L^{-1}	Soil-specific parameter
Organic matter content	f_{omfc}	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, *CL,TWA*, is calculated according the formula 10 but

with *CL, peak* instead of *CT, 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 are averaged	t_{avg}	days	7; 14; 21; 28; 56 days
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 $A_{met,2}$

Parameter	Symbol	Unit	Default values/Input
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 default scenario adjustment factor f_s and model adjustment factor f_M

Default scenario adjustment factors f_s

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

Default scenario adjustment factors f_s are used when performing an assessment for one of the PERSAM crops, included in the table of the FOCUS crops, for the three regulatory zones and for the concentration in total soil and for the concentration in pore water.

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: Default scenario adjustment factors f_s for PERSAM 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

Model adjustment factors f_M

Model adjustment factors f_M 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 f_M in soil according to email from EFSA to VITO dated 2 September 2013 is as follows:

- Model adjustment factor f_M = 2.0 for concentrations in total soil
- Model adjustment factor f_M = 4.0 for concentration in pore water

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

The model adjustment factors f_M 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 dependent on the zone and endpoint

	Symbol	Unit
Parameter		
Temperature T_{Arit}	T_{Arit}	K
Temperature T_{Arr}	T_{Arr}	K
Volumetric water content	.	$m^3\ m^{-3}$
Dry bulk density	.	$Kg\ L^{-1}$
Organic matter content	f_{om}	$kg.kg^{-1}$
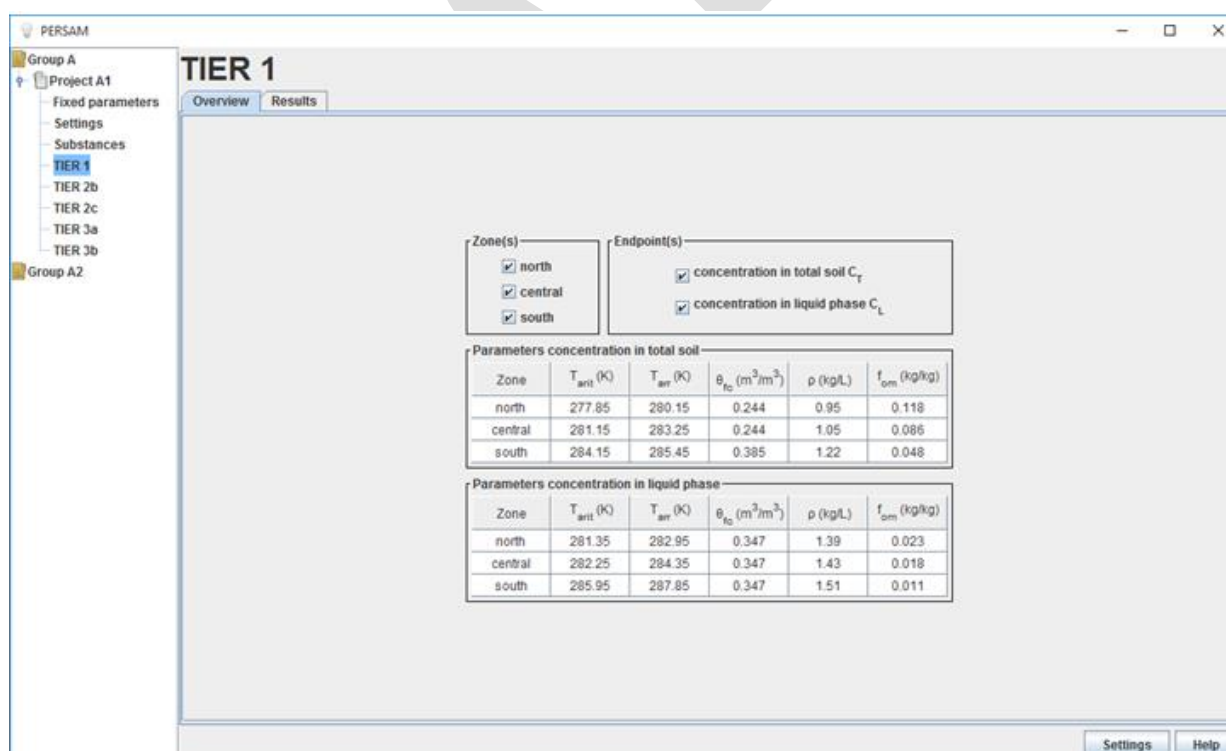
Figure 49:   TIER-1 overview tab

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.
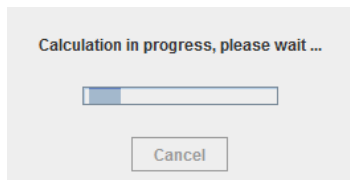
Figure 50:   Calculation in progress

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

Other functionalities:

o   Delete the results

o   Create a PDF report of the results

o   Export the results to a CSV file
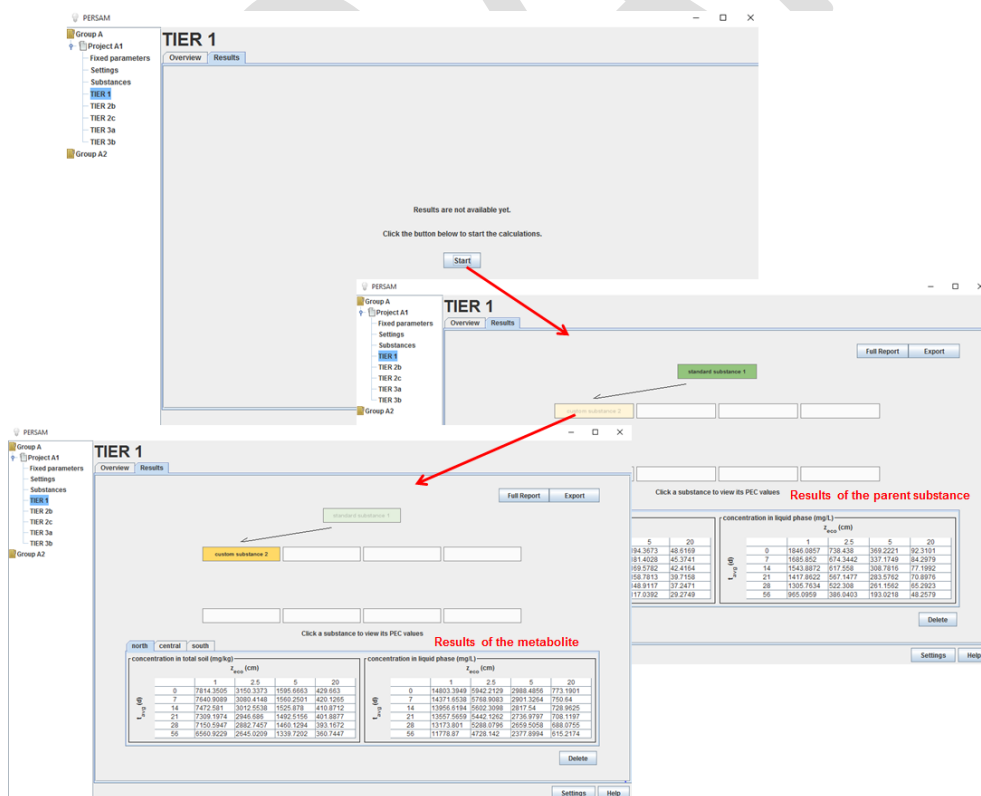
Figure 51:   Results of TIER-1

9. TIER-2B

TIER-2B is used to calculate the 95th-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 95th percentile can be selected. In TIER-2B, it suffices to calculate the 95th spatial percentile of the PEC of the required type of concentration.

The TIER-2B section is shown in following figure.
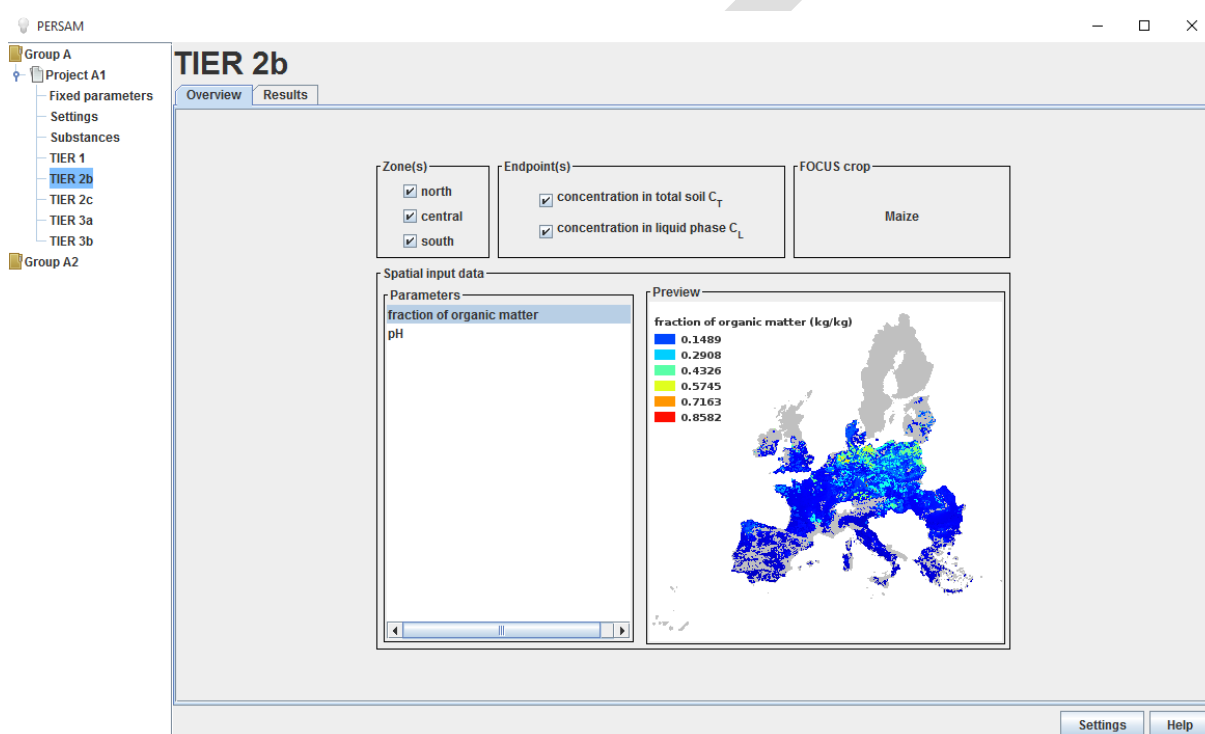
Figure 52:   TIER-2B section

9.1.   TIER-2B settings

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

- o   Zone(s) (see settings section)

- o   Endpoint(s) (see settings section)

- o   FOCUS crop (see settings section)

- o   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 (FOCUS 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 95th 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:

    o Fraction of organic matter
    o pH
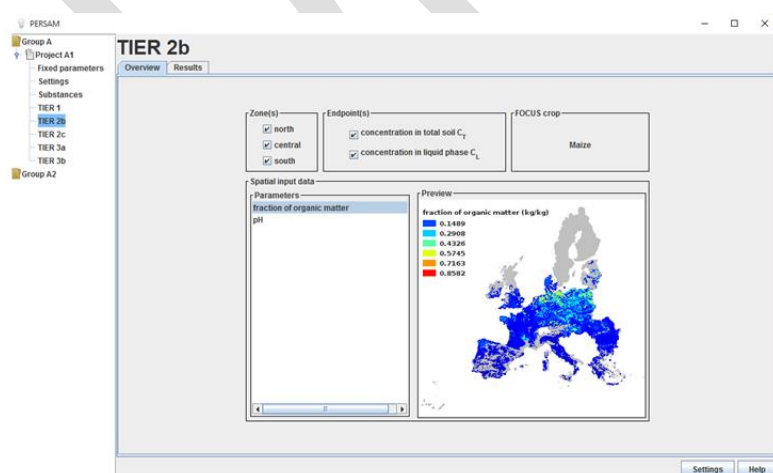
Figure 53: TIER-2B overview tab

In cases the selection of the FOCUS crops is spring cereals (not further specified) or winter cereals (not further specified), for the concentration in the total soil the application should use oats for the North Zone, rye for the Central Zone and common wheat for the South Zone. For the concentration in pore water, rye should be used for the North Zone, common wheat for the Central Zone and oats for the South Zone.

Therefore the overview window of TIER-2B presents different spatial input data.
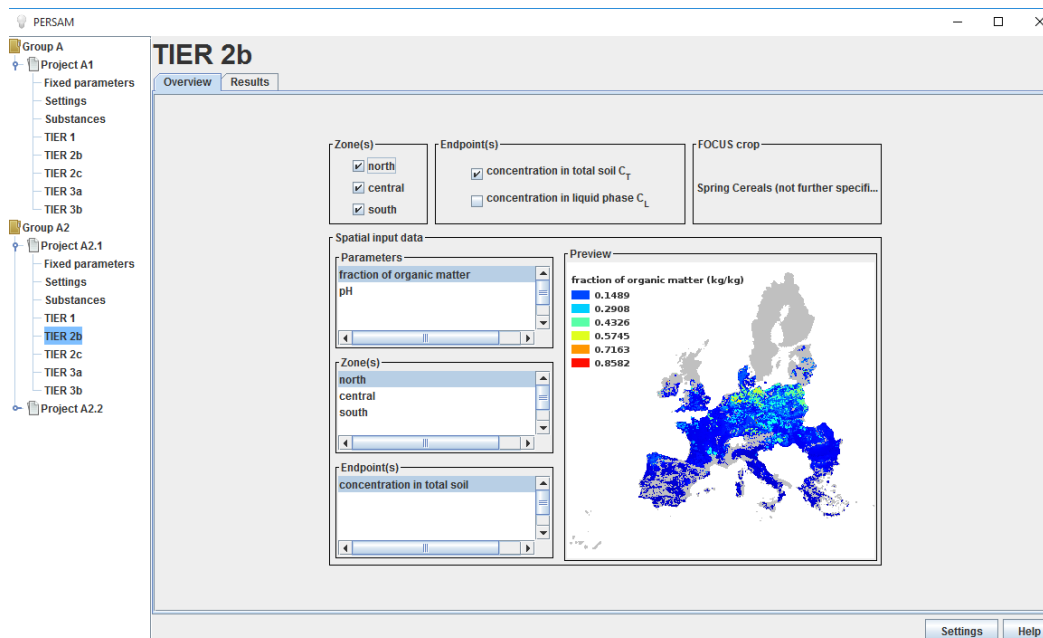
Figure 54:   TIER-2B overview tab for FOCUS crop 'Spring Cereals (not further specified)'

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 95th spatial percentile of calculated PECs for the regulatory selected zone with the related cumulative distribution graph and map.

Other functionalities:

  o   Delete the results

○ [Create a PDF report](#) of the results

○ [Export the results](#) to a CSV file

Figure 55: 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.
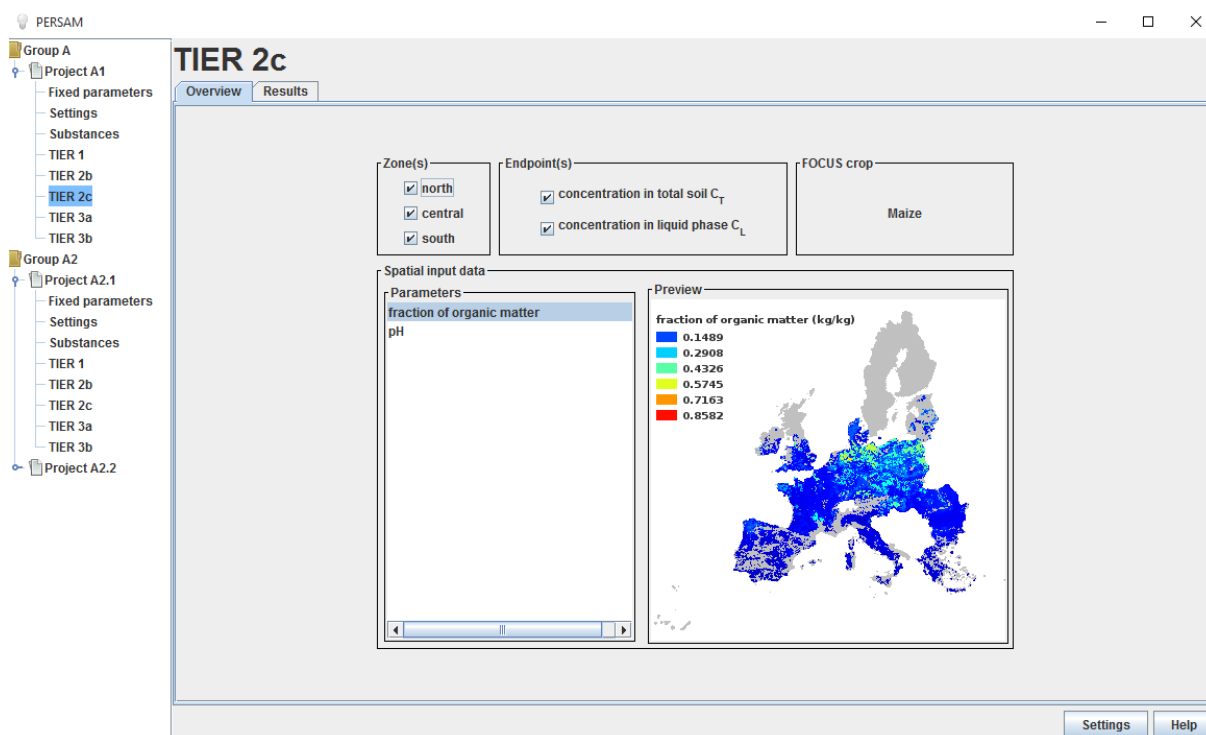
Figure 56:   TIER-2C section

10.1.   TIER-2C settings

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

- o   Zone(s) (see settings section)

- o   Endpoint(s) (see settings section)

- o   FOCUS crop (see settings section)

- o   Substances (parent & metabolites) (see substance section)

- o   Fraction that reached the soil ($F_{soil,\,max}$) (see settings section & substance 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:

- o   Fraction of organic matter
- o   pH
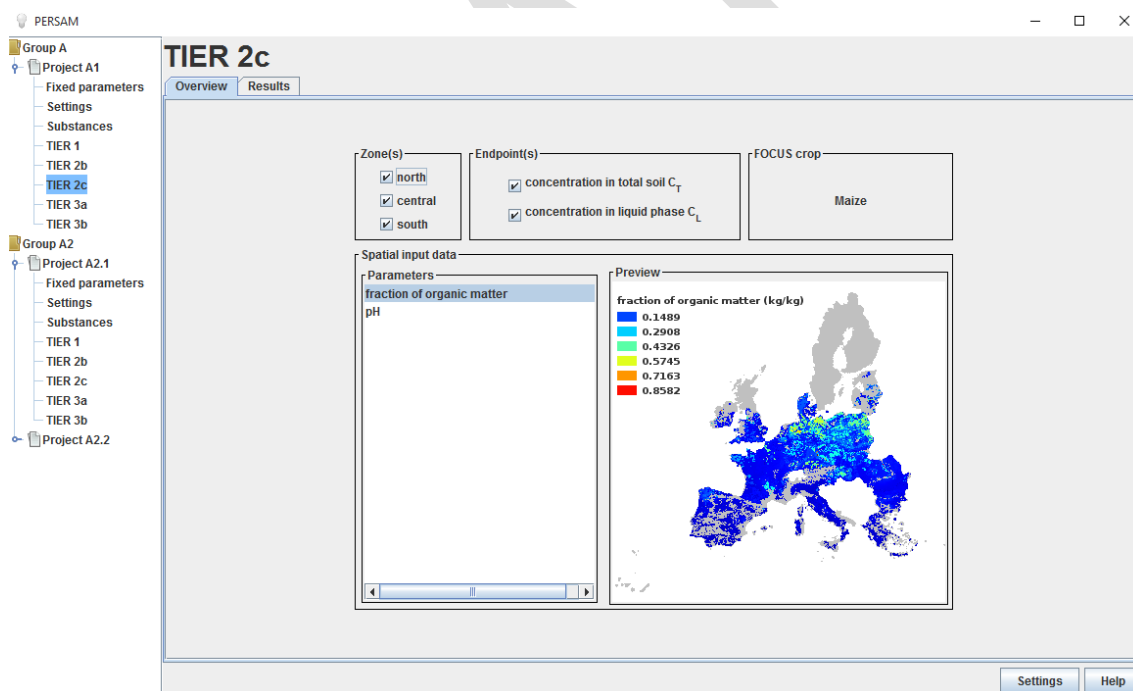
Figure 57:   TIER-2C overview tab

In cases the selection of the FOCUS crops is spring cereals (not further specified) or winter cereals (not further specified), for the concentration in the total soil the application should use oats for the North Zone, rye for the Central Zone and common wheat for the South Zone. For the concentration in pore water, rye should be used for the North Zone, common wheat for the Central Zone and oats for the South Zone.

Therefore the overview window of TIER-2C presents different spatial input data.
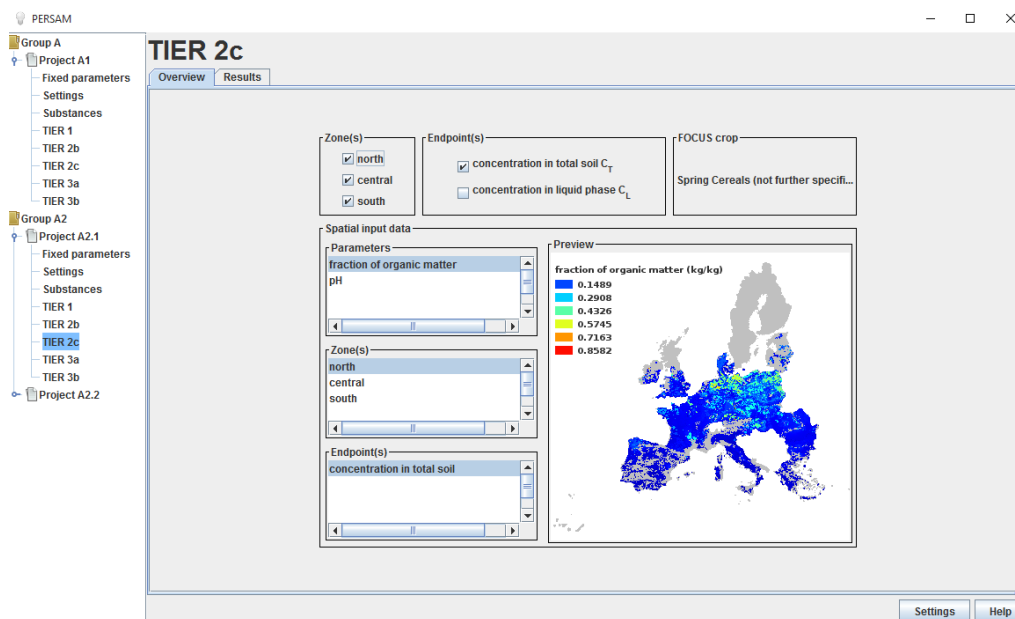
Figure 58:   TIER-2C overview tab for FOCUS crop 'Spring Cereals (not further specified)'
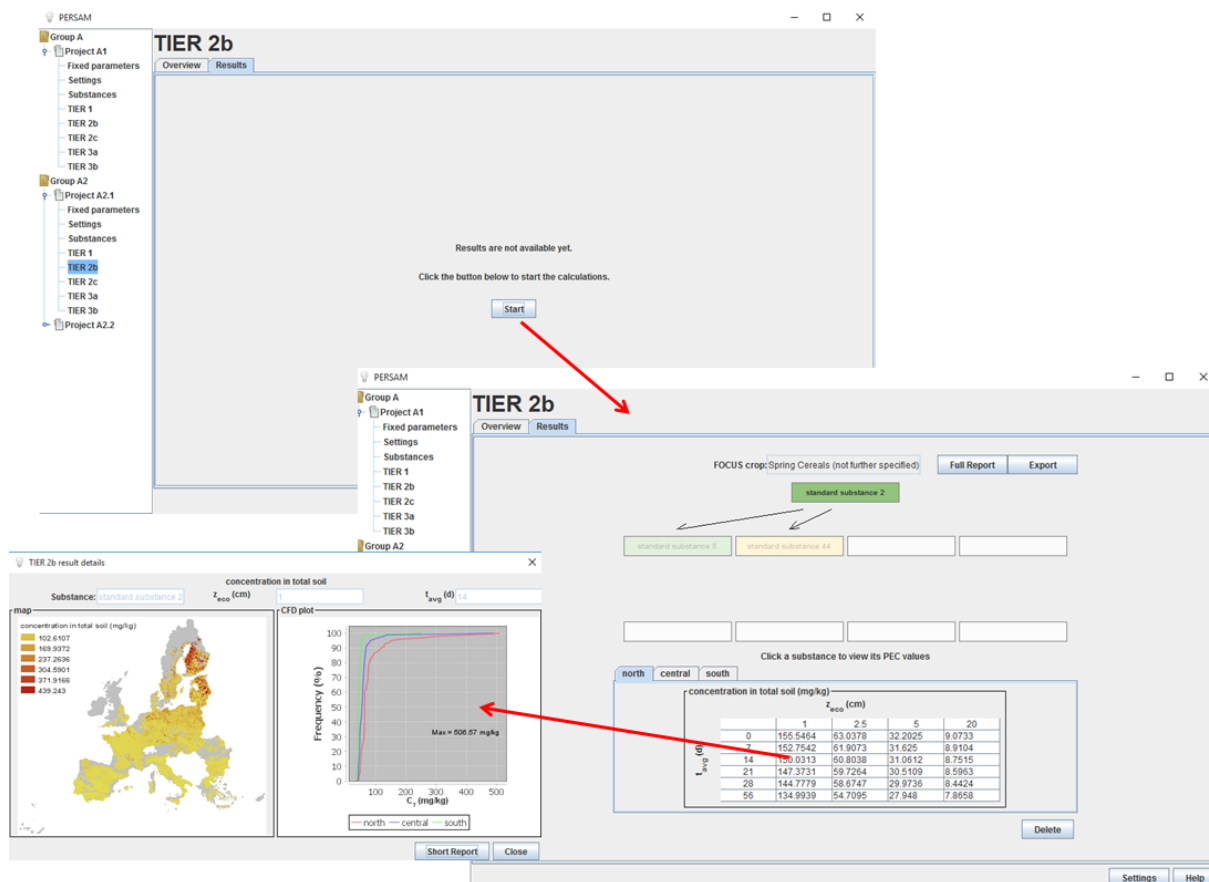
10.4.   TIER-2C results

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 95th 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-3A

PERSAM calculates the refines scenario adjustment factors based on the results of TIER-1 and TIER-2B.

The TIER-3A section is shown in following figure.
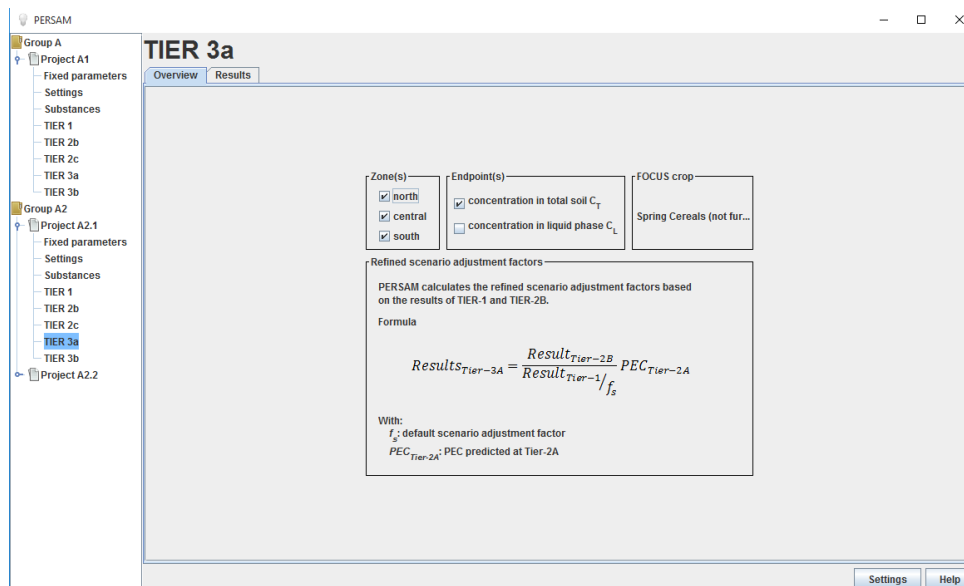
Figure 59:   TIER-3A section

11.1.   TIER-3A settings

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

- o   Zone(s) (see settings section)

- o   Endpoint(s) (see settings section)

- o   FOCUS crop (see settings section)

- o   Substances (parent & metabolites) (see substance section)

11.2.   TIER-3A calculations

PERSAM calculates substance- and crop-specific scenario adjustment factors to be used in Tier-3A assessments for a specific PERSAM crop.

The approach can be summarized as:

$$Results_{Tier-3A} = \frac{Result_{Tier-2B}}{Result_{Tier-1}/f_s} PEC_{Tier-2A}$$

where *ResultTier-1* is the result from the Tier 1 calculation, *fs* is the default scenario adjustment factor, *ResultTier-2B* is the result from Tier-2B, *PECTier-2A* is the PEC predicted at Tier-2A (without the scenario adjustment factor) and *ResultTier-3A* is the result for the Tier-3A assessment. The PERSAM output is the refined scenario adjustment factor circled in red.

11.1.   TIER-3A overview

The overview tab shows the configured settings that will be used in the calculations.
All parameters are not editable.
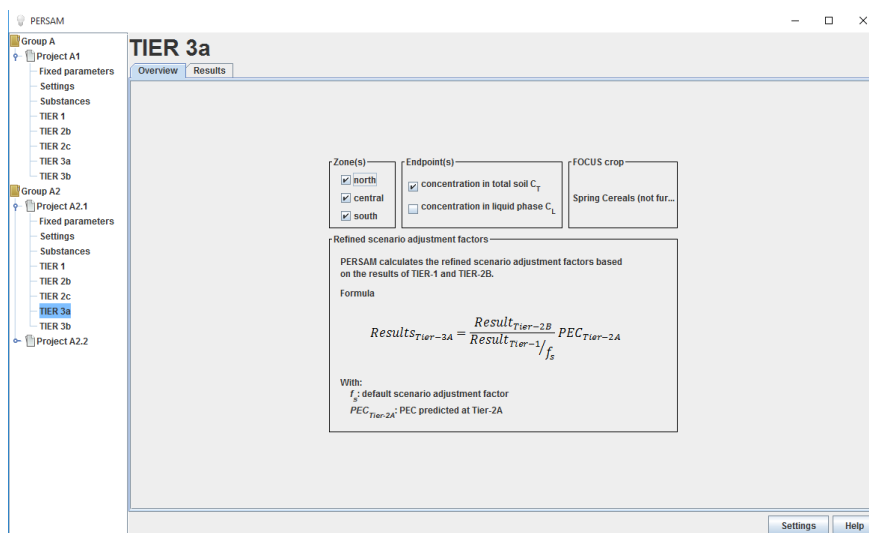
Figure 60:   TIER-3A overview tab

11.2.   TIER-3A 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-3B contains a table with the calculated refined scenario adjustment factors.


Other functionalities:

- o   Delete the results
- o   [Create a PDF report](#) of the results
- o   [Export the results](#) to a CSV file

Figure 61:   TIER-3A results tab

12.   TIER-3B

TIER-3 is designed to select the grid cell including the scenario properties corresponding to the 95th-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.
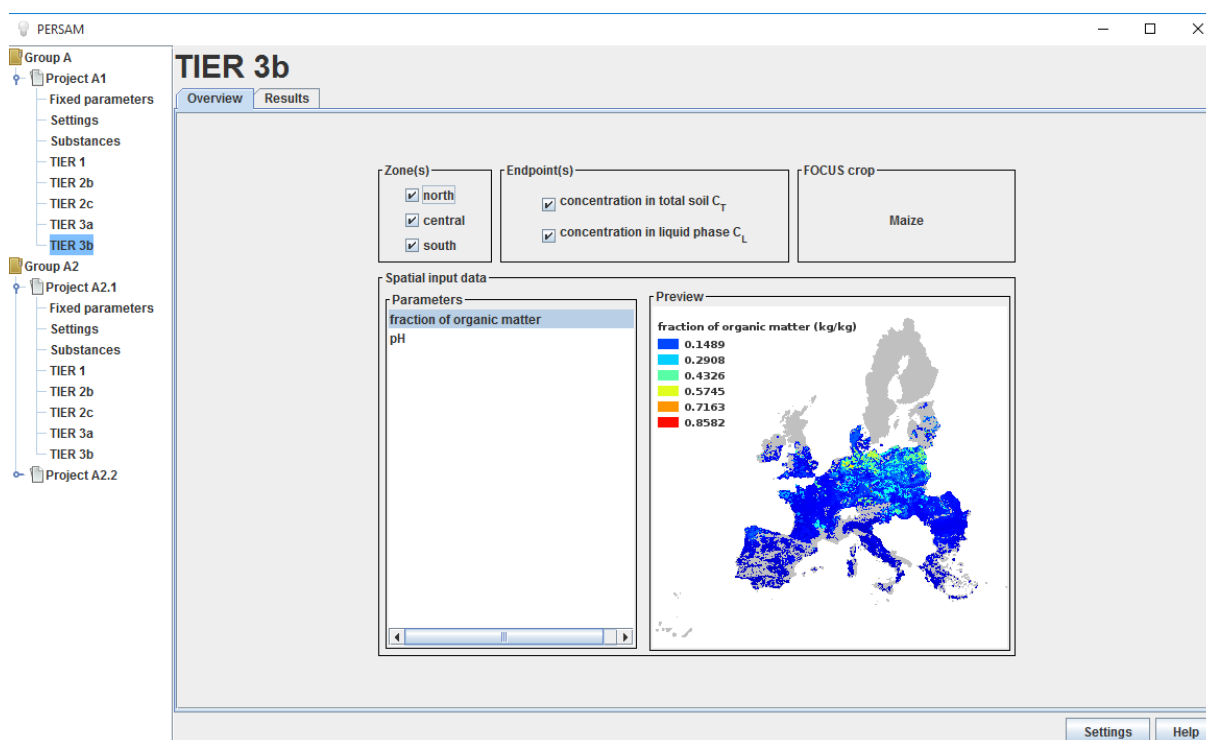
Figure 62:   TIER-3B section

12.1.   TIER-3B settings

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

- o   Zone(s) (see settings section)

- o   Endpoint(s) (see settings section)

- o   FOCUS crop (see settings section)

- o   Substances (parent & metabolites) (see substance section)

12.2. TIER-3B 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 95th 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. *CL,peak* or *CT, peak* or any of the TWA concentrations for *zeco* of 1, 2.5, 5 or 20 cm) and for the *DegT50 - Kom* 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 km2 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.

12.3. 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:

- o Fraction of organic matter
- o pH
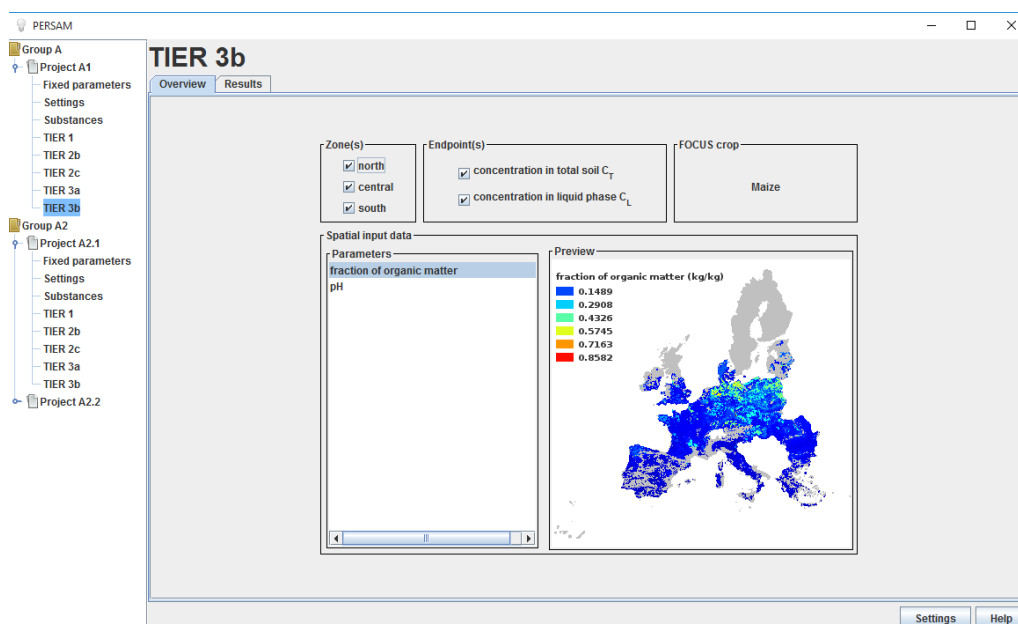
Figure 63:   TIER-3B overview tab

In cases the selection of the FOCUS crops is spring cereals (not further specified) or winter cereals (not further specified), for the concentration in the total soil the application should use oats for the North Zone, rye for the Central Zone and common wheat for the South Zone. For the concentration in pore water, rye should be used for the North Zone, common wheat for the Central Zone and oats for the South Zone.
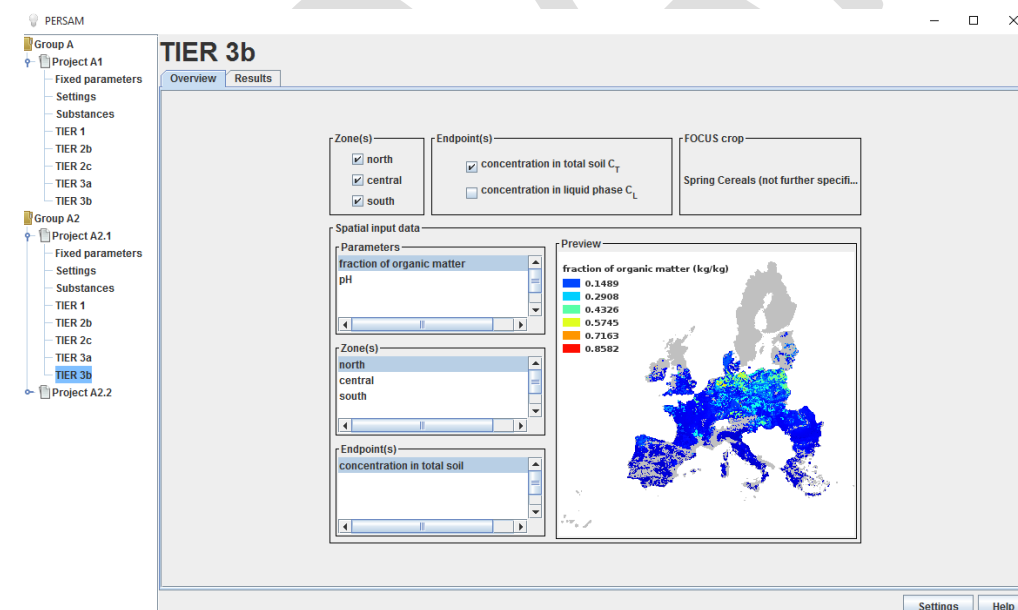
Figure 64:   TIER-3B overview tab for FOCUS crop 'Spring Cereals(not further specified)'

12.4.   TIER-3B 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:

- o Delete the results
- o [Create a PDF report](#) of the results
- o [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.
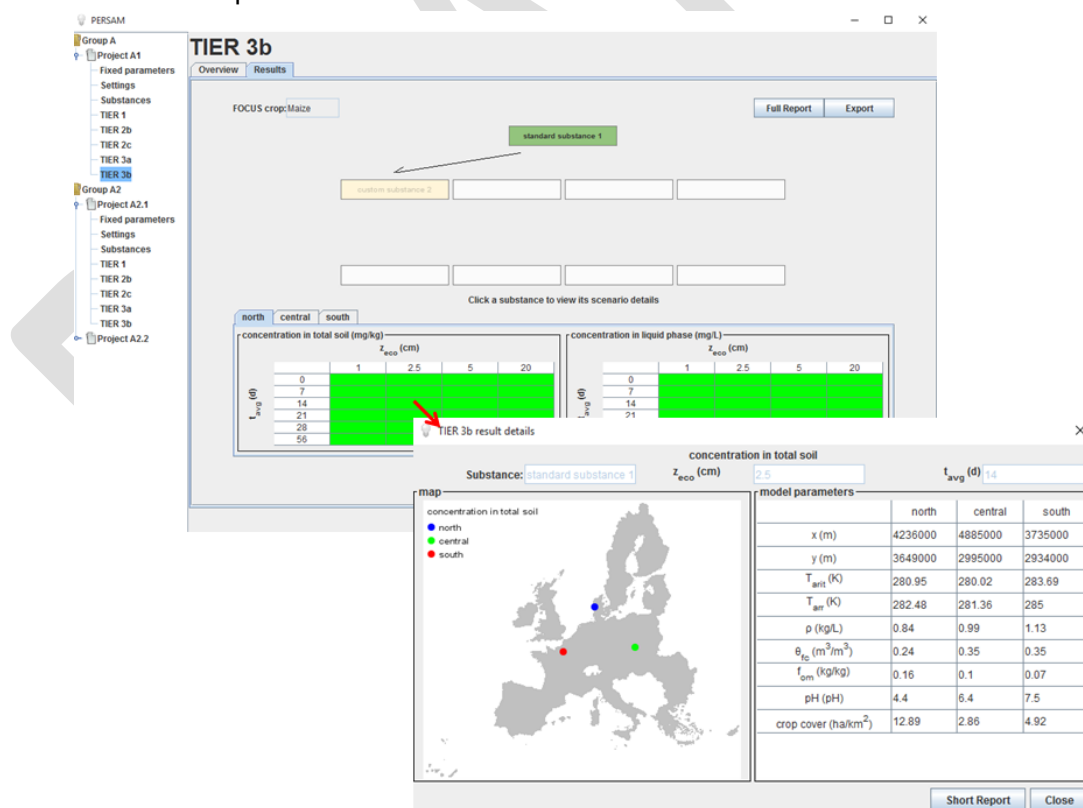
Figure 65:   Results of TIER-3B

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.

13.   Batch processing

All the calculations are automatically batch runs. This means when a user starts calculation, the calculation will run on the background
and the user has the possibility to work further on other projects. The advantage of batch processing is that the user can start several calculations
and he leaves his pc unattended, PERSAM will continue with the calculations.

How can I see that the calculation is still running on the background?
In the results tab you can see if the calculation still running in the batch queue.
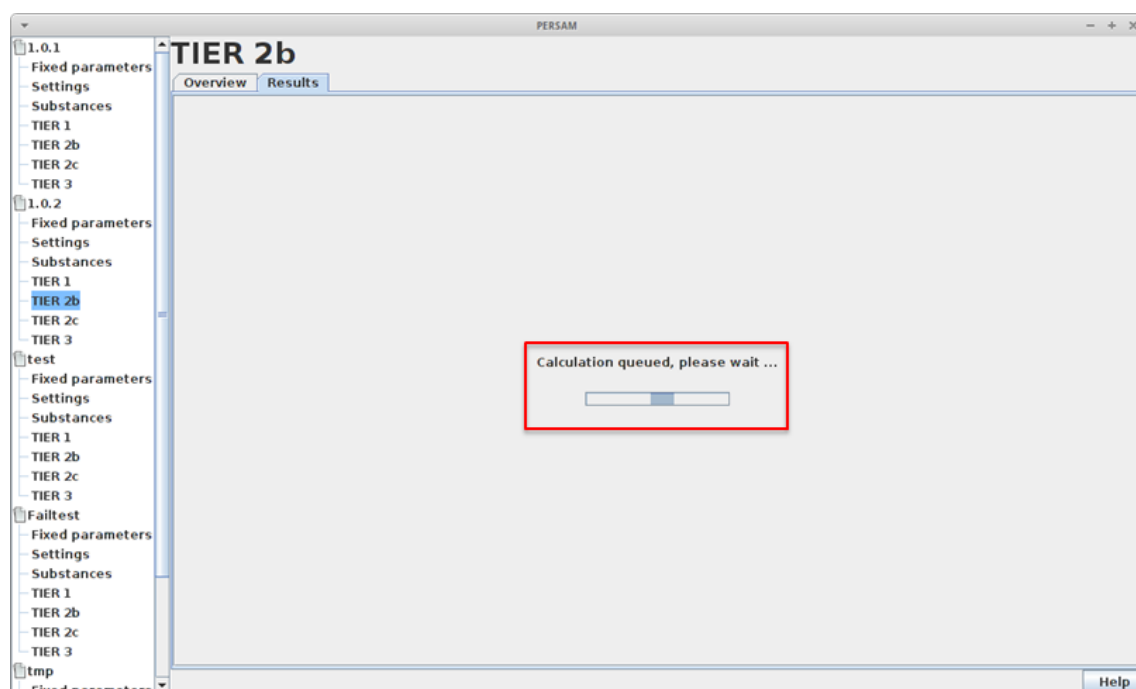
Figure 66:   Batch processing – calculations are still running

Can I change settings when I started a calculation in the batch queue?
When the calculation is still in the batch queue, you cannot change any setting of the project. The settings screen is disabled.
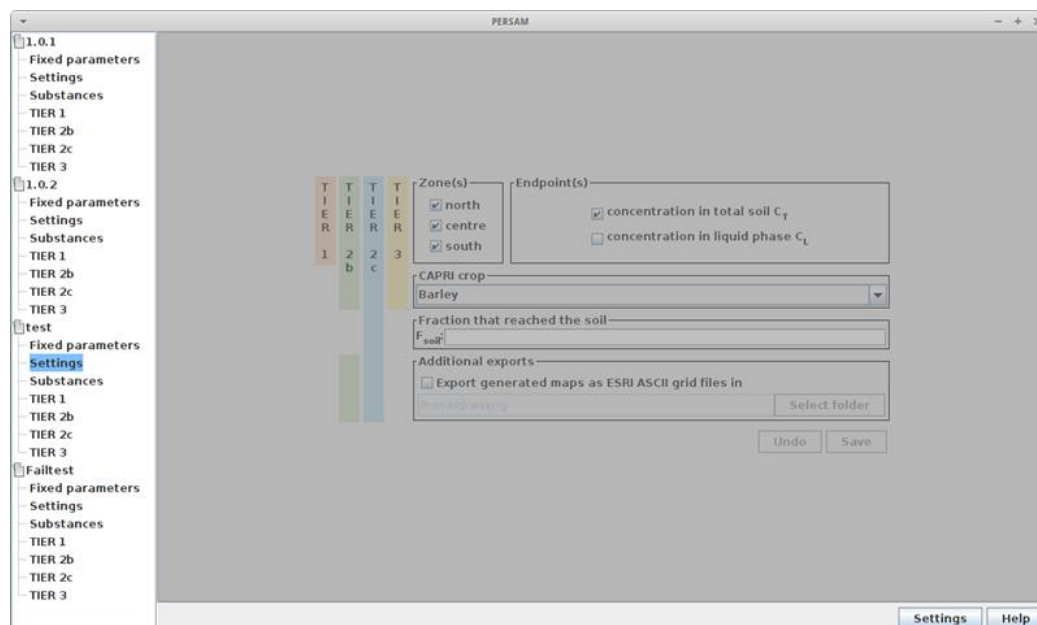
Figure 67:   Batch processing – settings screen is disabled

What happens if the calculation went wrong?

When there are problems in the batch processing with a particular calculations, the results tab gives the message 'Something went wrong, check log file'.

You can find the log file 'PERSAM.log' in the directory where you've installed the PERSAM software.
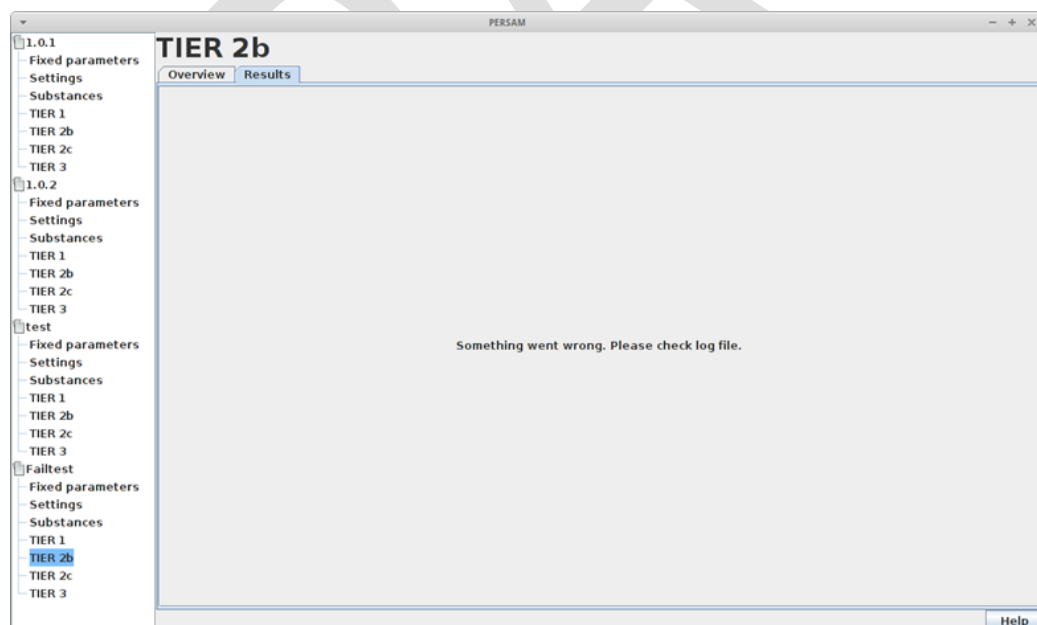
Figure 68:   Batch processing – problems during the batch processing

What happens when I close PERSAM and there are still calculations in the batch queue?

When you closes PERSAM and there are still calculations running, PERSAM will generate one of the following messages:
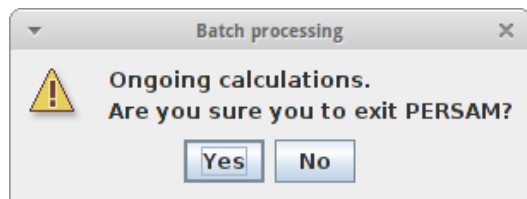
If you click on 'Yes', the calculations stays in the batch queue so that next time PERSAM can continue with the calculations.

If you closes PERSAM and there are unsaved changes, PERSAM will give next message:

What happens when I open PERSAM and there are still calculations in the batch queue?

When you opens PERSAM and there are still calculations waiting in the batch queue, PERSAM will give following message:
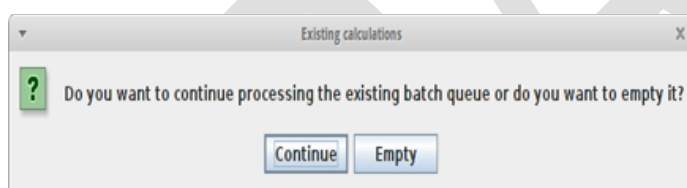
When there are failed calculations in the batch queue, PERSAM generates the message 'The batch queue contains some failed calculations.
Do you want to start with recalculations? Yes/No'.

14.   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.

14.1.   Automatic report generation

PERSAM has an option for automatically generate reports for short reports and full reports.

1. Click on the 'Settings' button in the main screen

2. Select the flag 'Automatically generate full reports' or 'Automatically generate short

    reports'

3. Define the reports output folder

4. Click on 'Save
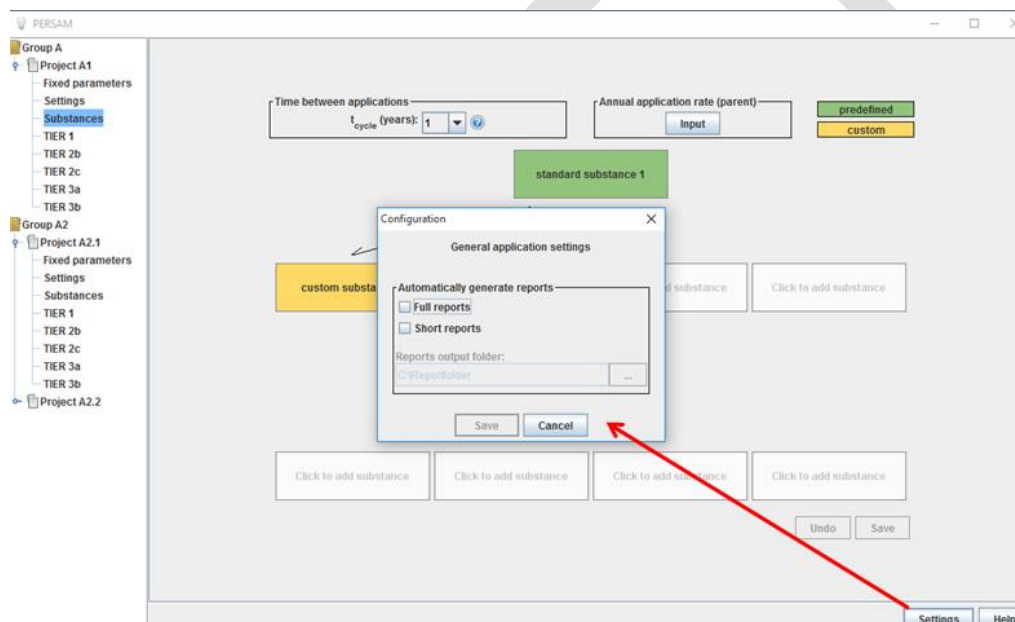
Figure 69:   Option: Automatically generate full reports and/or short reports

14.2.   Reporting

14.2.1. Full report

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

1. Go to the results tab of a particular TIER

2. Click on 'Full 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.
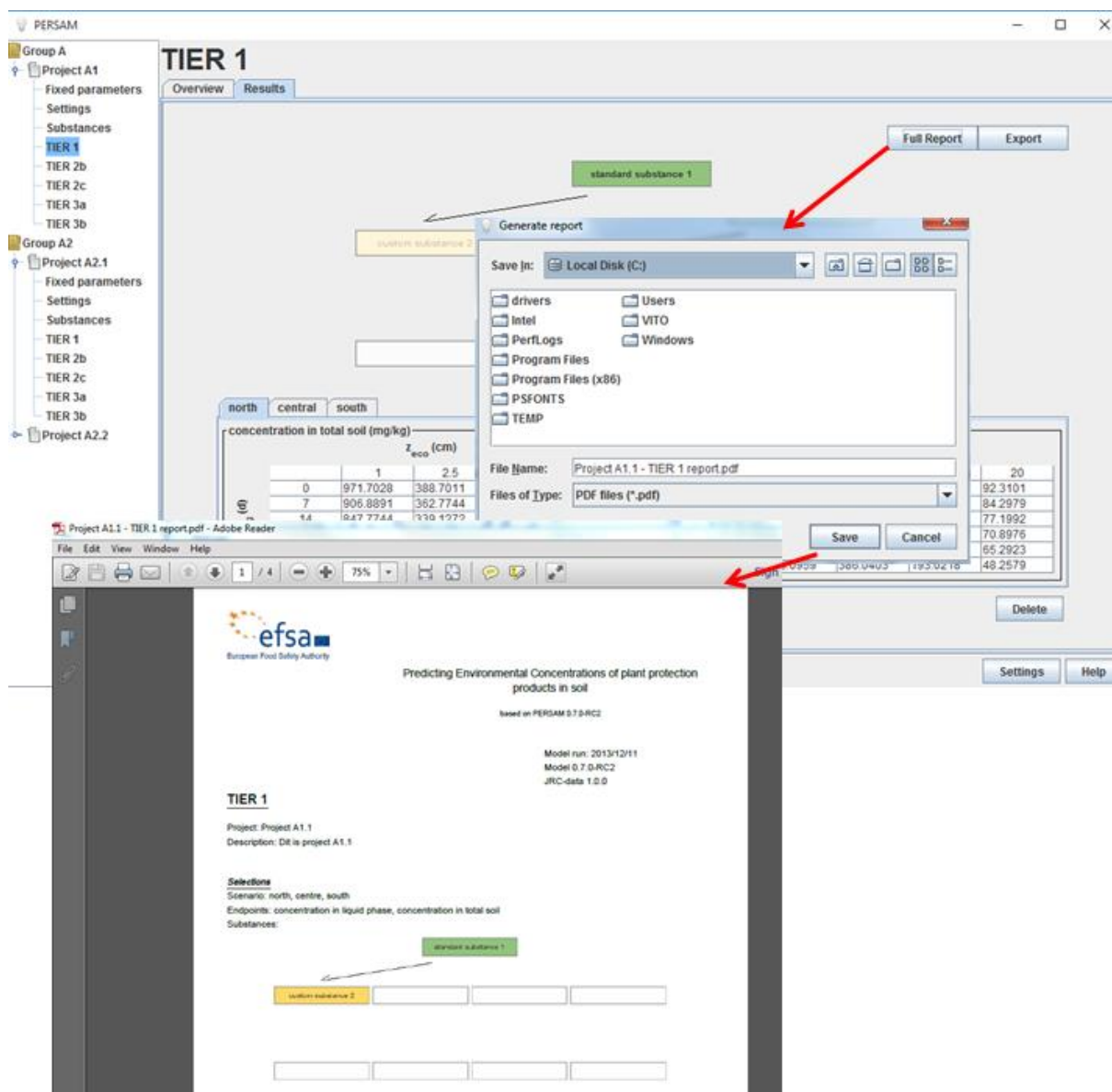
Figure 70:   Full report

14.2.2. Short report

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

1. Go to the results tab of a particular TIER

2. Go to the reports detail window and click on 'Short 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 for the selected Z_{eco} and T_{avg}

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 71:   Short report

14.3.   Export results

PERSAM provides the functionality to export the results of TIER-1, TIER-2B, TIER-2C, TIER-3A and TIER-3B 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.
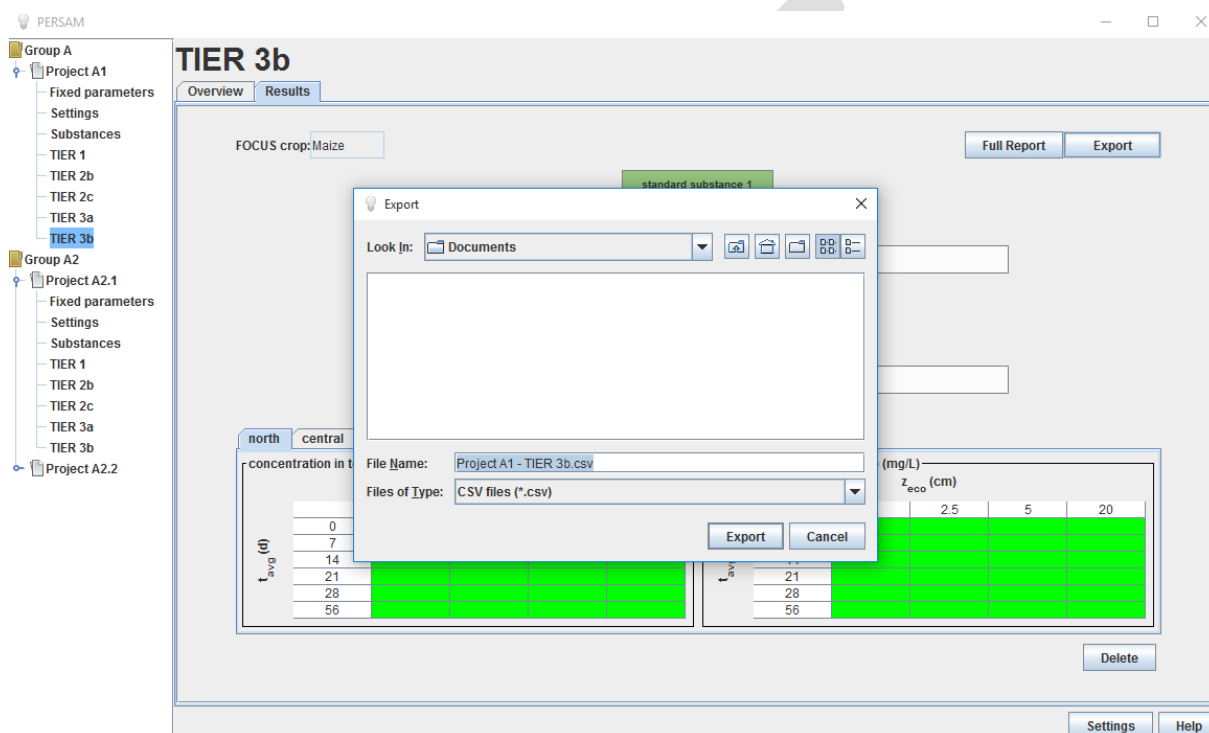
Figure 72:   Exporting results

15.   Additional information

This section contains additional information such as:

- o   [FOCUS Crops](#)
- o   [EFSA Spatial version](#)

15.1.   FOCUS Crops

Next table contains the FOCUS crop list.

Table 13: FOCUS crops

FOCUS crop	PERSAM crop	CTN	CTC	CTS	CLN	CLC	CLS
Beans (field)	Pulses	HA	HA	–	HA	HA	–
Beans (vegetables)	Pulses	–	–	PO	–	–	TH
Cabbage	Other fresh vegetables	JO	CH	KR	HA	CH	SE
Carrots	Other fresh vegetables	–	CH	KR	HA	CH	TH
Cotton	Texture crops	–	–	SE	–	–	SE
Linseed	Texture crops	–	OK	OK	–	OK	OK
Maize	Maize	HA	CH	KR	HA	CH	SE
No crops (= fallow soil)	Fallow	JO	CH	KR	HA	CH	SE
Oil seed rape (summer)	Oilseed rapes	JO	OK	–	JO	OK	–
Oil seed rape (winter)	Oilseed rapes	HA	CH	KR	HA	CH	PI
Onions	Other fresh vegetables	JO	CH	KR	HA	CH	TH
Onions	Floriculture and flower bulbs[a]	JO	CH	KR	HA	CH	TH
Peas (animals)	Pulses	JO	CH	–	HA	CH	–
Potatoes[b]	Potatoes	JO	CH	KR	HA	CH	TH
Soybean	Soya beans	–	PI	PI	–	PI	PI
Strawberries	Other fresh vegetables	JO	HA	KR	HA	HA	SE
Sugar beets	Sugar beets	JO	CH	KR	HA	CH	SE
Sunflower	Sunflowers	–	PI	PI	–	PI	SE
Tobacco	Tobacco	–	–	PI	–	–	TH
Tomatoes	Other fresh vegetables	–	CH	PI	–	CH	SE
Spring cereals[c]	Barley	JO	CH	KR	HA	CH	PO
	Common wheat	JO	CH	KR	HA	CH	PO
	Durum wheat	–	CH	KR	–	CH	PO
	Oats	JO	CH	KR	HA	CH	PO
	Rye	JO	CH	KR	HA	CH	PO
Winter cereals[c]	Barley	JO	CH	KR	HA	CH	SE
	Common wheat	JO	CH	KR	HA	CH	SE
	Durum wheat	–	CH	KR	–	CH	SE
	Oats	JO	CH	KR	HA	CH	SE
	Rye	JO	CH	KR	HA	CH	SE

(a): Not a FOCUS crop; therefore, onions are suggested as a surrogate in the numerical models at Tiers 2A, 3A and 3B.
(b): Potatoes are included in PERSAM; however, this guidance document does not apply to crops grown on ridges.
(c): In cases where the FOCUS crop spring or winter cereals is not represented by a PERSAM crop or is not further specified, for the concentration in the total soil, the application should use oats for the North Zone, rye for the Central Zone and common wheat for the South Zone. For the concentration in the pore water, rye should be used for the North Zone, common wheat for the Central Zone and oats for the South Zone. These crops have the largest scenario adjustment factors in their respective regulatory zones (also refer to Tables C.2 and C.3).
CH, Châteaudun; HA, Hamburg; JO, Jokioinen; KR, Kremsmünster; OK, Okehampton; PI, Piacenza; PO, Porto; SE, Seville.
See EC (2014) for further details.

15.2.   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/

16.   Troubleshooting and Helpdesk

Troubleshooting during the installation procedure:

- o   ***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

- o   ***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:

- o   What is your operating system and version number?
- o   Where is the PERSAM directory located: on the disk of your pc or on a network disk?
- o   Do you have administrator rights on your pc? If not, what rights do you have?
- o   Please, give a detailed description of the different steps you've done before the problem popped up.
- o   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.

EFSA, 2012a. European Food Safety Authority; Tier-1 and Tier-2A Scenario Parameterisation and Example Calculations. EFSA Journal 2012;10(1):2433 [64 pp.]. doi:10.2903/j.efsa.2012.2433.

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.

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

Opinion of the Scientific committee/scientific panel, Question number: EFSA-Q-2012-00299, EFSA Journal 2012;10(2):2562 [76 pp.]. doi:10.2903/j.efsa.2012.2562

EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. Question number: EFSA-Q-2012-00877, EFSA Journal 2015;13(4):4093. Doi: 10.2903/j.efsa.2015.4093

Outcome of the public consultation on the draft EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil, Question number: EFSA-Q-2013-00076

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})
$DegT_{50}$	Degradation half-life in soil (days)
ρ	Dry bulk density of the soil (kg.dm^{-3})
E	Arrhenius activation energy
f_M	Model adjustment factors
f_{om}	Organic matter content (-)
f_S	Default scenario adjustment factors
f_{soil}	Fraction that reaches the soil (-)
K_{om}	Organic matter/water distribution coefficient (L.kg^{-1})
M	Molar mass
R	Gas constant
T_{arit}	Arithmetic mean temperature (K)
T_{arr}	Arrhenius weighted average soil temperature (K)
t_{avg}	Averaging time
t_{cycle}	Time between applications
T_{ref}	Reference temperature
θ_{fc}	Water content at field capacity (m^3.m^{-3})
z_{eco}	Ecotoxicological averaging depth
z_{til}	Plough depth

Appendix A – FOCUS Crops[1]

FOCUS crop	PERSAM crop	CTN	CTC	CTS	CLN	CLC	CLS
Beans (field)	Pulses	HA	HA	–	HA	HA	–
Beans (vegetables)	Pulses	–	–	PO	–	–	TH
Cabbage	Other fresh vegetables	JO	CH	KR	HA	CH	SE
Carrots	Other fresh vegetables	–	CH	KR	HA	CH	TH
Cotton	Texture crops	–	–	SE	–	–	SE
Linseed	Texture crops	–	OK	OK	–	OK	OK
Maize	Maize	HA	CH	KR	HA	CH	SE
No crops (= fallow soil)	Fallow	JO	CH	KR	HA	CH	SE
Oil seed rape (summer)	Oilseed rapes	JO	OK	–	JO	OK	–
Oil seed rape (winter)	Oilseed rapes	HA	CH	KR	HA	CH	PI
Onions	Other fresh vegetables	JO	CH	KR	HA	CH	TH
Onions	Floriculture and flower bulbs[a]	JO	CH	KR	HA	CH	TH
Peas (animals)	Pulses	JO	CH	–	HA	CH	–
Potatoes[b]	Potatoes	JO	CH	KR	HA	CH	TH
Soybean	Soya beans	–	PI	PI	–	PI	PI
Strawberries	Other fresh vegetables	JO	HA	KR	HA	HA	SE
Sugar beets	Sugar beets	JO	CH	KR	HA	CH	SE
Sunflower	Sunflowers	–	PI	PI	–	PI	SE
Tobacco	Tobacco	–	–	PI	–	–	TH
Tomatoes	Other fresh vegetables	–	CH	PI	–	CH	SE
Spring cereals[c]	Barley	JO	CH	KR	HA	CH	PO
	Common wheat	JO	CH	KR	HA	CH	PO
	Durum wheat	–	CH	KR	–	CH	PO
	Oats	JO	CH	KR	HA	CH	PO
	Rye	JO	CH	KR	HA	CH	PO
Winter cereals[c]	Barley	JO	CH	KR	HA	CH	SE
	Common wheat	JO	CH	KR	HA	CH	SE
	Durum wheat	–	CH	KR	–	CH	SE
	Oats	JO	CH	KR	HA	CH	SE
	Rye	JO	CH	KR	HA	CH	SE

(a): Not a FOCUS crop; therefore, onions are suggested as a surrogate in the numerical models at Tiers 2A, 3A and 3B.
(b): Potatoes are included in PERSAM; however, this guidance document does not apply to crops grown on ridges.
(c): In cases where the FOCUS crop spring or winter cereals is not represented by a PERSAM crop or is not further specified, for the concentration in the total soil, the application should use oats for the North Zone, rye for the Central Zone and common wheat for the South Zone. For the concentration in the pore water, rye should be used for the North Zone, common wheat for the Central Zone and oats for the South Zone. These crops have the largest scenario adjustment factors in their respective regulatory zones (also refer to Tables C.2 and C.3).
CH, Châteaudun; HA, Hamburg; JO, Jokioinen; KR, Kremsmünster; OK, Okehampton; PI, Piacenza; PO, Porto; SE, Seville. See EC (2014) for further details.

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[1] See EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal 2015;13(4):4093, 102 pp., doi:10.2903/j.efsa.2015.4093

Appendix B − Soil-specific parameters[2]

Total concentration in soil

Properties of the predefined scenarios used at TIER-1, TIER-2B and TIER-3A for the concentration in total soil.

Zone	Code	Country	T_{arit} [(a)] (°C)	T_{arr} [(b)] (°C)	Texture	f_{om} (−) [(c)]	θ_{fc} (m³ m⁻³) [(d)]	ρ (kg dm⁻³) [(e)]
North	CTN	Estonia	4.7	7.0	Coarse	0.118	0.244	0.95
Central	CTC	Germany	8.0	10.1	Coarse	0.086	0.244	1.05
South	CTS	France	11.0	12.3	Medium fine	0.048	0.385	1.22

(a): T_{arit} is the arithmetic mean annual temperature
(b): T_{arr} is the Arrhenius-weighted mean annual temperature (explained in EFSA PPR Panel, 2012a)
(c): f_{om} (−) is the organic matter content
(d): θ_{fc} (m³ m⁻³) is the water content at field capacity
(e): ρ (kg dm⁻³) is the dry bulk density of the soil.
Soil properties are those of the top 30 cm of the soil, for properties of the other soil layers refer to EFSA PPR Panel (2012b)

CTC, scenario for the total concentration in the Central Zone; CTN, scenario for the total concentration in the North Zone; CTS, scenario for the total concentration in the South Zone.

Concentration in liquid phase

Properties of the selected predefined scenarios used at TIERS 1, 2A and 3A for the concentration in pore water.

Zone	Code	Country	T_{arit} [(a)] (°C)	T_{arr} [(b)] (°C)	Texture	f_{om} (−) [(c)]	θ_{fc} (m³ m⁻³) [(d)]	ρ (kg dm⁻³) [(e)]
North	CLN	Denmark	8.2	9.8	Medium	0.023	0.347	1.39
Central	CLC	Czech Republic	9.1	11.2	Medium	0.018	0.347	1.43
South	CLS	Spain	12.8	14.7	Medium	0.011	0.347	1.51

(a): T_{arit} is the arithmetic mean annual temperature
(b): T_{arr} is the Arrhenius-weighted mean annual temperature (explained in EFSA PPR Panel, 2012a)
(c): f_{om} (−) is the organic matter content
(d): θ_{fc} (m³ m⁻³) is the water content at field capacity
(e): ρ (kg dm⁻³) is the dry bulk density of the soil.
Soil properties are those of the top 30 cm of the soil, for properties of the other soil layers refer to EFSA PPR Panel (2012b)

CLC, scenario for the concentration in pore water for the Central Zone; CLN, scenario for the concentration in pore water for the North Zone; CLS, scenario for the concentration in pore water for the South Zone.

Appendix C − Substance - specific parameters[3]

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

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

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[3] See EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal 2015;13(4):4093, 102 pp., doi:10.2903/j.efsa.2015.4093