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# 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 95<sup>th</sup>-percentile PEC's
- ✓ TIER-2C 95<sup>th</sup>-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 95<sup>th</sup>-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.

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**Key words:** Exposure assessment, soil, plant protection products, soil organisms, ecotoxicological effects, tiered approaches, crop interception, Help file, Persistence in Soil Analytical Model (PERSAM), PERSAM

## Question number: EFSA-Q-2016-00265

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# Summary

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

The aims and objectives of the project are to develop a software tool for calculating the predicted environmental concentrations of substances and their transformation products in soil in support of the EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. The tool will be based on an analytical model for which both the concepts and the mathematical equations are described in the Scientific Opinion (EFSA, 2012b), and in the EFSA Guidance document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances 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 95<sup>th</sup>-percentile PEC's
- TIER-2C 95<sup>th</sup>-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 95<sup>th</sup>-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

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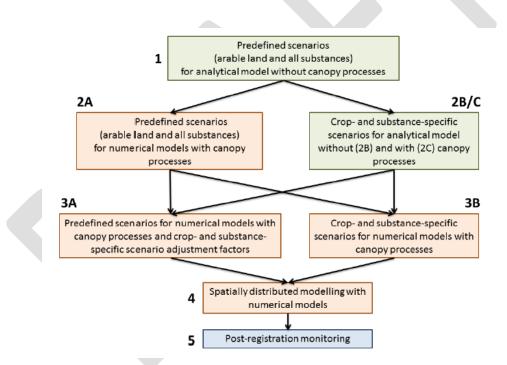


# **1.2.** Interpretation of the Terms of Reference

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

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<sup>7</sup> 



described in the opinion. More specifically, the software tool will be able to calculate:

- ✓ TIER-1 Predicted Environmental concentrations
- ✓ TIER-2B 95<sup>th</sup>-percentile PEC's
- ✓ TIER-2C 95<sup>th</sup>-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 95<sup>th</sup>-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
- $\checkmark$  The user can enter application rate(s), application time and Fsoil for multiple applications
- ✓ TIER-3A
- ✓ Batch processing

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# 2. Tutorial

Use the Tutorial for a quick start with the application.

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

# 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





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#### 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

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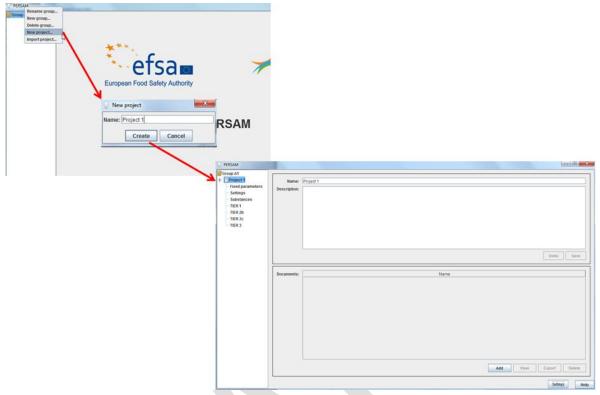
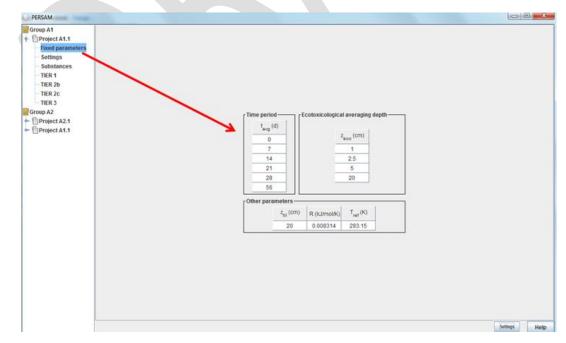


Figure 4: Project management – Create a new project

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

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



## Figure 5: Fixed parameters

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## 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'

PERSAM		-		×
Group A				
👇 📋 Project A1				
<ul> <li>Fixed parameters</li> </ul>				
Settings				
Substances				
TIER 1				
TIER 2b				
TIER 2c	T T T T Zone(s) [Endpoint(s)]			
TIER 3a				
TIER 3b	E E E E E			
Group A2				
	1 2 2 3 3 V south			
	b c a b FOCUS crop			
	Spring Cereals (Common wheat)			
	spring cerears (common wheat)			
	TIER 2c-			
	Calculate TIER 2c			
	r Additional exports			
	Export generated maps as ESRI ASCII grid files in			
	C:\Users\\EUser Select folder			
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# 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
- Click on the 'Input' button for <u>defining the application rate(s)</u> for one or <u>multiple applications</u>. 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'

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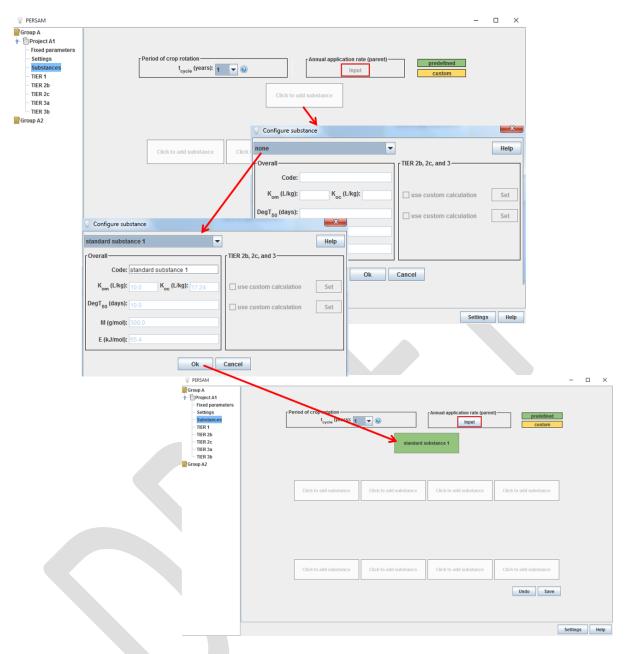


Figure 7: Configure a predefined substance (parent or metabolite)

#### 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'

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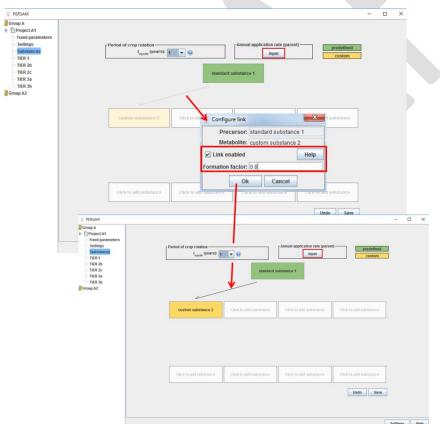
#### Additional information

- Define customized substances or metabolites: see <u>Configure custom substance</u>
- 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.
- 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?

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

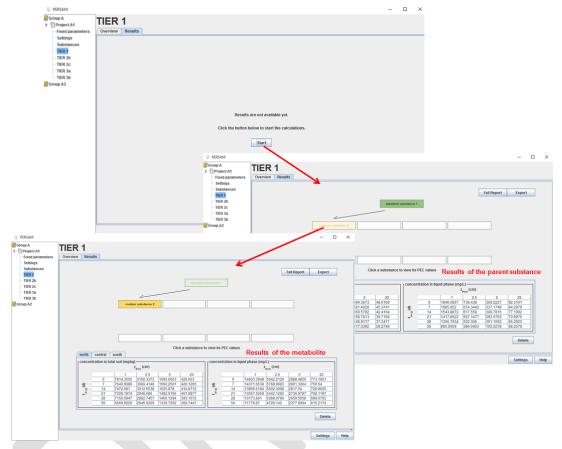


Figure 9: Results of TIER-1

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

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

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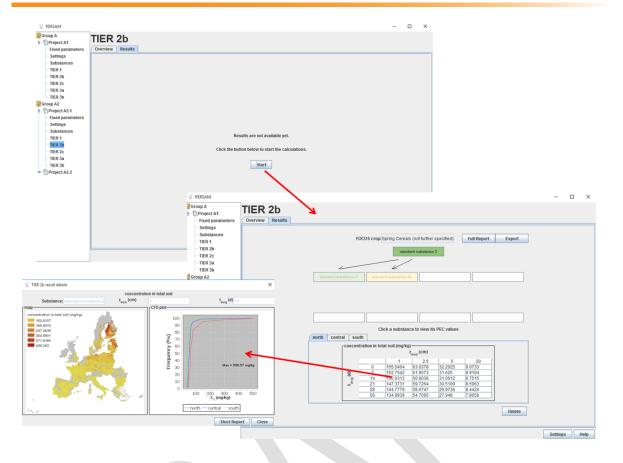


Figure 10: Results of TIER-2B

#### 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<sub>soil,max</sub>
- 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.
- Click on a cell in the table to view extended results. A detail window appears containing the 95<sup>th</sup> spatial percentile of calculated PECs for the regulatory selected zone with the related cumulative distribution graph and map.

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## 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.

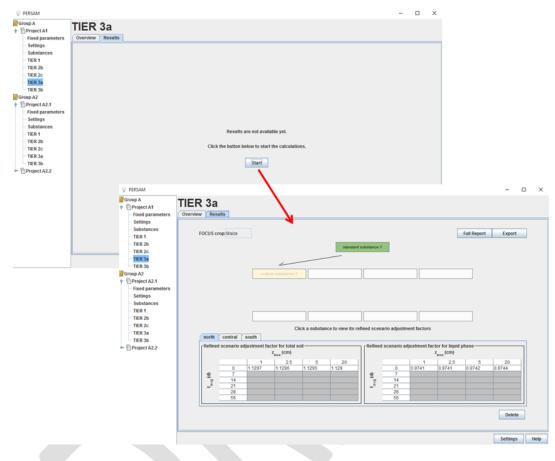


Figure 11: Results of TIER-3A

#### How can you perform the TIER-3 B calculations?

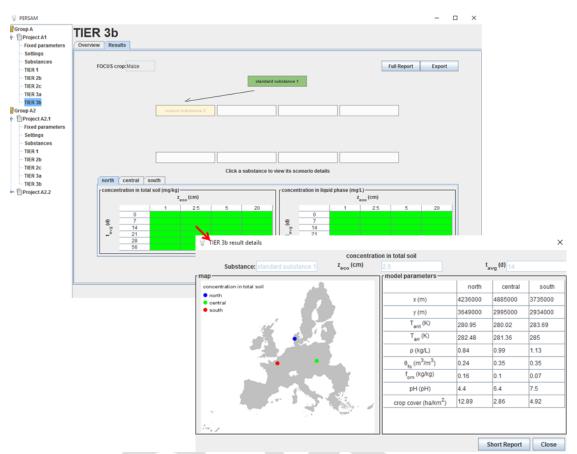
- 1. Go to the project tree and select 'TIER-3'
- 2. Go to the 'Results' tab
- 3. Select a substance in the Substance tree to view the results. The results tab of TIER-3 contains a table with the green cells which indicates whether there results are available
- 4. Click on a particular cell (a combination 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.

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#### 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.

**<u>Remark</u>**: 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.

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# <u>Tips</u>:

- Before you install a new version of PERSAM, <u>export</u> all your projects. After the installation you can <u>import</u> 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 <u>automatically generation of pdf reports</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

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# 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 (<u>http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/</u>) 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

- Start your browser and go to the JRC soil portal (<u>http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/</u>)
- 2. Download the software:
  - $\rightarrow$  Save the software on your computer and start the installation from your computer by double click on the executable
  - or
- $\rightarrow$  Start immediately the installation
- 3. If you have already PERSAM installed on your computer, you will get next message:



PERSAM seems to be already installed on your system. Would you like to remove the previous installation first? Note that this will also erase all your PERSAM projects.



Figure 13: Message 'PERSAM already installed'

 $\rightarrow$  Yes: all PERSAM projects will be erased

 $\rightarrow$  No: the installation won't start and you can <u>export</u> the PERSAM projects and <u>import</u> the projects after the installation.

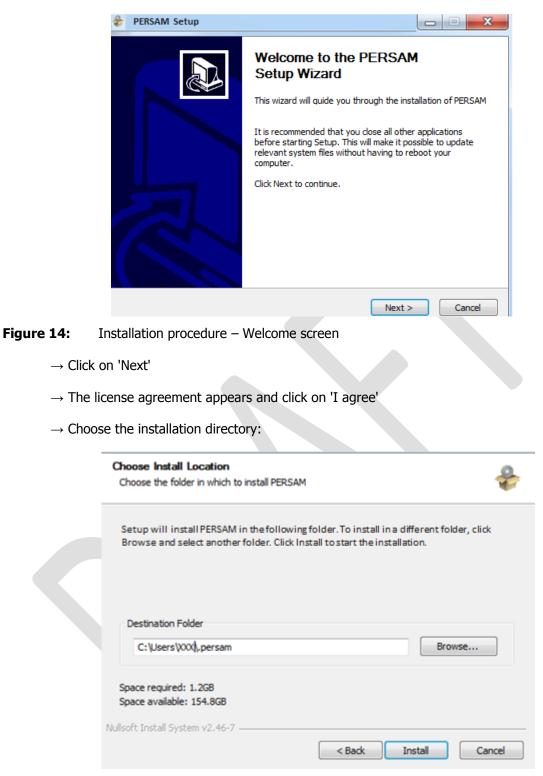
#### 4. Starting the installation procedure

```
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#### **Figure 15:** Installation procedure – Choose installation directory

- $\rightarrow$  Select the destination folder and click on 'Install'
- $\rightarrow$  The installation will start

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	🕹 PERSAM Setup	
	Installing Please wait while PERSAM is being installed.	÷
	Extract: maize.dat	
	Nullsoft Install System v2.46-7	Cancel
Figure 16	Installation procedure – Installing the software	

- $\rightarrow$  After the installation, click on 'Finish'
- 5. You can find the PERSAM application in the start menu of your computer:

R	Snipping Tool
Ì	Paint
	XPS Viewer
9	PERSAM
•	All Programs

Figure 17: PERSAM application in start menu

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# **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 <u>http://eusoils.jrc.ec.europa.eu/library/Data/EFSA</u>

# 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?

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

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





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# 4.1. Group

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

# **Related functionalities:**

- o <u>New group</u>
- o <u>Rename group</u>
- o <u>Delete group</u>

#### 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'



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#### 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'

PERSAM Rename group. New group. Delete group. New project Import project	Rename group Old name: Group 1 New name: Group A1 Rename Cancel	y Authority	VITO vision on techn
		PERSAM	PERSAM
			efsa a
			PERSAM
gure <b>21</b> : Ren	ame 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.

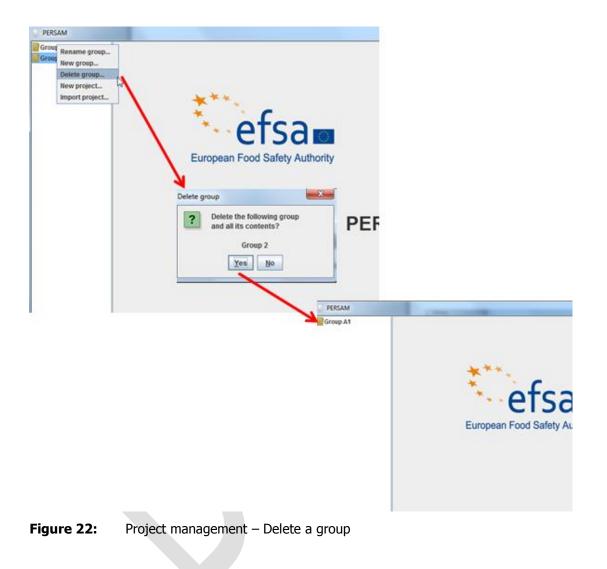
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- 3. Following message appears: Delete the following group and all its contents?
  - Yes: delete the selected group
  - No: don't delete the selected group



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# 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: <u>fixed parameters</u>, <u>settings</u>, <u>substances</u>, <u>TIER-1</u>, <u>TIER-2B</u>, <u>TIER-2C</u>, <u>TIER-3A</u> and <u>TIER-3B</u>.

roup A1			
Project A1	Name	Deliand.	
FIGULAT		e: Project A1	
	Description		
		Undo	Sa
	Documents	s: Name	
		Map1.xisx	
		Add View Export	Delet

Figure 23: Project main screen

#### Documents

The user can <u>add</u> relevant documents to the project.

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

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#### **Related project functionalities:**

- o <u>New project</u>
- o <u>Rename project</u>
- o <u>Copy/Paste project</u>
- o <u>Delete project</u>
- o Import project
- o <u>Export project</u>

## 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'

Reserved And and Broom- Development of Service- There property Here property European Food Safety Authority	
New project Name: Project 1 RSAM Create Cancel PRSAM Create Cancel PRSAM Createsex	Name: Proved 1
- 1984 - 1982 - 1982 - 1982 - 1983	Documents
	Add Vers Expert Delete



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## 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'

V PERSAM	
Group A1  Fixed parameters  Substances  TER 1  TER 2b  TER 2b  TER 2b  TER 3c	Name: [Projed 1 Description:
Croup A1  Croup A1  Croup A1  Croup A1  Fixed parameters  Substances  TER 1  TER 25  TER 25  TER 3	Name: PopedAt 5 Description: Undo Save
	And

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.

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💡 PERSAM	
Group A1 - Fixed par - Settings - Substanc - TIER 1 - TIER 2b - TIER 2c - TIER 3 Group A2	Cription: Dit is project A1.1
	Documents:

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'

F S S S S S S S S S S S S S S S S S S S	European F Fixed param Settings Group A1 Project A1.1 Fixed param Settings Group A2 TER 2 TER 2 Group A2 Fixed param Settings	eters Description:	Project A1.1 Dtl is project A1.1	
9	- Substances - TER 1 - TER 2b - TER 2c - TER 3	Documents:		Name

Figure 27: Project management – Past project

5. Rename the project

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## 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

Project A Project te Fixed pa		
Fixed pa Settings Substances TIER 1	roject	
TIER 2b TIER 2c TIER 3	Delete project	
	Delete the following project?	
	Project test Yes No Docume	
		ERSAM roup A1  Project A1.1
		*
		Euro

Figure 28: Project management – Delete project

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# 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 <u>export</u> 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.

<u>Note:</u> If you import a project from a previous version of PERSAM, the current version of PERSAM takes the first FOCUS crop of the <u>FOCUS crop list</u> where PERSAM crop corresponds with CAPRI crop from the imported project.

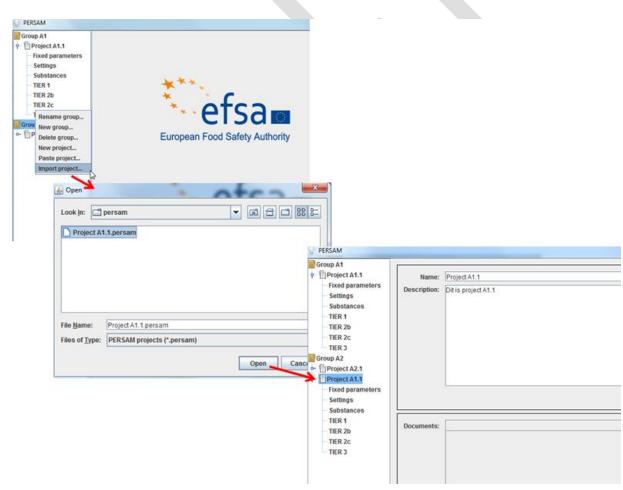


Figure 29: Project management – Import project

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## 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 <u>import</u> 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.

PERSAM			
Group A1 Copy project Project A1 Export project Copy project Export project Delete project Settings Substances - TIER 1 - TIER 2b - TIER 2c	Name: Project A ription: Dit is pro		×
Froject A2.1		persam	
	File <u>N</u> ame: Files of <u>T</u> ype:	Project A1.1.persam PERSAM projects (*.persam)	Save Cancel

**Figure 30:** Project management – Export project

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#### 4.2.7. Document management

The user can <u>add</u> relevant documents to the project.

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

Next document types are supported:

- o Excel
- $\circ$  Word
- o PDF
- o TXT
- o CSV

Group A1  Fixed parameters Settings Substances TIER 1 TIER 2b TIER 2c TIER 3 Group A2  Project A2.1 Project A1.1		Project A1.1 Dit is project A1.1 Undo Save
	Documents:	Name Add View Export Delete
	Docum	nentmanagement

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.

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				le le			
the second se	c Project A1 1						
Description	Dit is project A1.1						
				Undo	Saw		
Documents		Name					
	Book1.xlsx						
	PERSAM.docx PERSAM.pdf						
	data.csv						
	data bi						
	-						
			Add	/iew Export	Delete		
				Expose			
			have been a second s	N			
				~			
			T PERSAMpdr - Adobe Read	~			
			File Edit Vew Window	Help			
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			File Edit Vew Window	Help		0012	3
			File Edit Vew Window	Help		0012	
			File Edit Vew Window	Help		<b>00</b>   <b>7</b>	
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				Help 1 + 1 / 1 - 4	• 201% • E	rtical Model (PERSAM) av	sists the user in
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			Tét Lét Van Winder	top () () () () () () () () () () () () () (	Persistence in Soil Anal Persistence in Soil Anal ing the analytic model, to calculate control PEC's centile PEC's centile PEC's	ytical Model (PERSAM) av as desembed in the optimon out from TIER-2A simulatio ff, and	sists the user in More specifically, the ms with numerical
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			To Let Vee Worker	http 1 (1) (1) (1) (1) (1) (1) (1) (1) (1) (1	10% + E E	steal Model (PERSAM) as as described in the option pot from TER-2A simulation ff, and no properties corresponding not of TER-3	usts the user in More specifically, the one with numerical g to the 95 <sup>th</sup> percentile
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Figure 32:

Document management – Add document

#### **View document**

The user can view the documents related to the project.

- 1. Select a particular document
- 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

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### **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'

PERSAM						- • • •×
Group A1						
e- Project A1.1	Name:	Project A1.1				
- Fixed parameters		Dit is project A1.1				
- Settings	Description:	Dit is project A1.1				
- Substances						
- TIER 1						
- TIER 2b						
- TIER 2c						
TIER 3						
Group A2						
← ① Project A2.1						
► Project A1.1						
					Undo	Save
					01110	0410
i i i i i i i i i i i i i i i i i i i						
	Documents:			Name		
		Book1.xlsx				
		PERSAM.docx PERSAM.pdf				
		data.csv				
		data.bt				
		💡 Save		×		
		Save In: 🗐	Local Disk (C:)	- 6 🗂 🗂 🐭 💳	Add View Export	Delete
L			-			
		drivers	C Users			
		intel	CTIV C			
		PerfLogs	C Windows			
		C Program F	iles 🗋 msdia80.dll			
		Program P	iles (x86) 🗋 PosteClient.log			
		C PSFONTS	STARTUP.LOG		<b>*</b>	
		TEMP				
		File Name:	data.csv			
		Files of Type:	All Files			
		thes of Table:		-		
				Save Cancel		
				Save Cancel		

Figure 34:Document management – Export document

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#### **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

PERSAM					- 0 <u>- ×</u>
Group A1					
- Project A1.1	Name:	Project A1.1			
<ul> <li>Fixed parameters</li> </ul>		Dit is project A1.1			
- Settings					
- Substances					
- TIER 1					
TIER 2b					
TIER 2c TIER 3					
Group A2					
- Project A2.1					
e- Project A1.1					
- Fixed parameters				-	
Settings					Undo Save
Substances					
- TIER 1	Documents:		Name		
- TIER 2b	Documents:	Book1.xlsx	Name		
- TIER 2c		data.csv			
TIER 3		data.txt PERSAM.docx			
		PERSAM.dock			
			Delete document		
			Delete document		
			Are you sure you want to delete		
			Are you sure you want to delete document 'Book1,xisx'?		
			OK Cancel		
				Add View E	xport Delete
Figure 35:	Docume	ent managemer	nt – Delete document		

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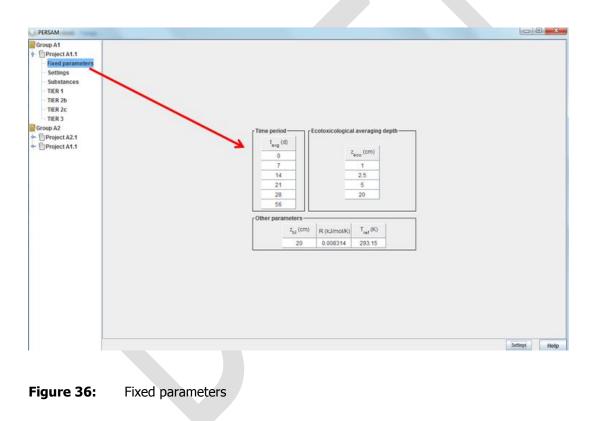
# 5. Fixed parameters

The fixed parameters section gives an overview of all parameters that are used

in the calculations but cannot be changed by the user.

#### Table 1: Fixed parameters

	Symbol	Unit	Default values
Parameter			
Ecotoxicological averaging depth	Z <sub>eco</sub>	cm	1; 2.5; 5; 20
Plough depth	Z <sub>til</sub>	cm	20
Gas constant	R	kJ.mol⁻¹.K⁻	0.008314
Reference temperature	T <sub>ref</sub>	ĸ	293.15
Time period since application over	t <sub>avg</sub>	days	0; 7; 14; 21; 28; 56



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# 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.

		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 <u>FOCUS crop list</u>	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.

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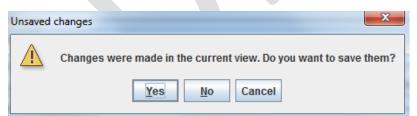
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💡 PERSAM							-		×
Group A Project A1 Fixed parameters Substances TIER 1 TIER 2b TIER 2c									
- TIER 3a	 T I	T T	T T	T T	T T	Zone(s) Endpoint(s)			
Group A2	ER	E	Ε	Ε	Ε	concentration in total soil C <sub>T</sub>			
Group A2	R 1	2	R 2		R 3				
		b		а		[FOCUS crop			
						Spring Cereals (Common wheat)			
						TIER 2c			
						Calculate TIER 2c			
						Additional exports			
						Export generated maps as ESRI ASCII grid files in			
						C:\Users\IEUser Select folder			
						Undo Save			
					0	pen 🖌 💌			
					Loc	ok In: 🗟 Local Disk (C:) 🔹 🖬 🗂 📴 📴			
						drivers 🔂 Users			
					_	Intel 🔄 VITO			
						PerfLogs  Windows Program Files	Setting	s	Help
						Program Files (x86)			
						PSFONTS TEMP			
						TEMP			
					Fol	der name: C:\			
					File	s of Type: All Files			
						Open Cancel			

## 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.

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• 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.

0			_	
PERSAM		-		×
Group A Project A1 Fixed parameters Substances TIER 1 TIER 2b TIER 2c TIER 3a TIER 3b Group A2	Time between applications t <sub>cycle</sub> (years): 1 • • • • • • • • • • • • • • • • • •			
	standard substance 4     standard substance 66     Click to add substance			
	Click to add substance Click to add substance Click to add substance Undo Save	Settings		-telp
		Settings		lelp

### 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.

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#### Table 3: Substance-specific parameters

	Symbol	Unit	Default value
Parameter			
Half life for degradation of the	DegT50	days	
Organic matter/water	K <sub>om</sub>	l/kg	
Organic carbon/water	K <sub>oc</sub>	l/kg	
Molar mass	Μ	g.mol <sup>-1</sup>	
Arrhenius activation energy	E	kJ.mol <sup>-1</sup>	65.4
Formation fraction metabolite	F <sub>f</sub>		
Annual application rate	А	kg/ha	

## **Related functionalities:**

- <u>Configure Application rate(s)</u>
- 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.

- 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.

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V PERSAM				- 0	×						
Group A	Period of crop rotation t <sub>cycle</sub> (years): 1 v @	Annual application rate (parent)	custom	]							
	Multiple applications	*			×						
	Number of applications										
	1 1 1 1 1 1 1 1 1 1 5 10	1                 15	1 1 1 20	<u>La 1</u> -1	25 30						
	Annual application rate A, (kg/ha)	Number of days from the first	t application	Fraction	that reaches the soil (f <sub>soil</sub> )						
	2.0	Ĵ	0		0.2						
	3.0		30		0.5						
	2.0	1	50		0.3						
		Ok Cancel	Help								

Figure 40: Multiple applications – Define application rate(s) & f<sub>soil</sub>

- 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.
- 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:**  $0 \le the value of fsoil \le 1$ 

 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

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6. Click 'OK'

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

1) Calculate residues in soil with: Rp;  $A_{i-1} * exp(-[ln(2)/DegT50] * t_i)$ (1)residues *i* remaining from previous applications *i*-1 (g/ha) (Rp<sub>1</sub> is set to 0)  $Rp_i$ : total actual application rate of app. no. i (g/ha)  $A_i$ : DegT50: half life of the substance at scenario temperature (d) time since the last application for application no i (d) t<sub>i</sub>: 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: = NA<sub>i</sub> \*  $f_{soil,i}$  + Rp<sub>i</sub> (2) A NA<sub>i</sub>: nominal application rate no. i in the sequence of applications (g/ha) f<sub>soil,i</sub>: fraction of application *i* reaching the soil (-) Rpi: 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<sub>i</sub>, f<sub>soil,1</sub> is not further used in the PERSAM calculation as it is already taken into account in the calculation of A<sub>i</sub>. PERSAM users must be able to give for each application A<sub>i</sub>, f<sub>soil,1</sub>, t<sub>i</sub>.

**<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'

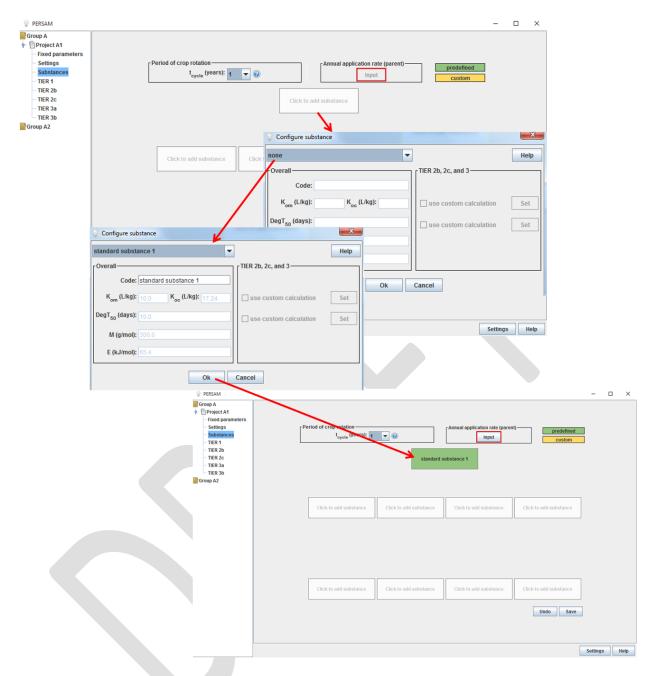
Note: If the user selects the code, the substance related parameters become editable and the user can <u>configure a customized substance</u>.

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

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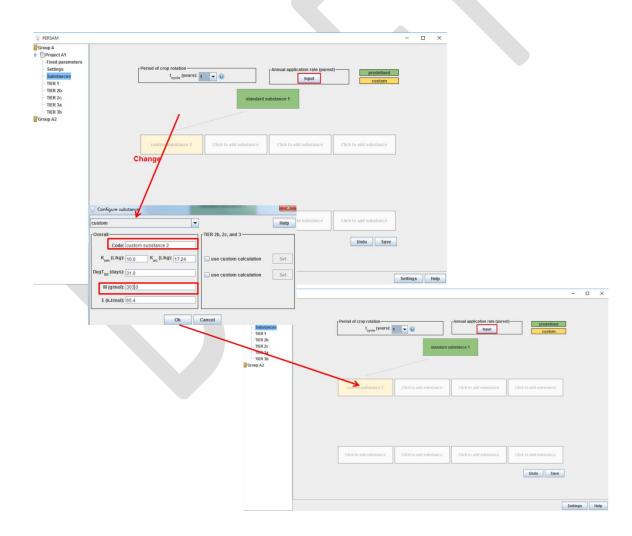


# 7.3. Configure custom substance

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

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#### 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.

Configure substance		x
custom	н	elp
Overall-	TIER 2b, 2c, and 3	
Code:		
K <sub>om</sub> (L/kg): K <sub>oc</sub> (L/kg):	use custom calculation S	et
DegT <sub>50</sub> (days):	use custom calculation	et
M (g/mol):		
E (kJ/mol): 65.4		
Ok	Cancel	

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.
- Configure a predefined substance (see <u>Configure predefined substance</u>) or a custom substance (see <u>Configure custom substance</u>)
- 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

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PERSAM							- 0	×	
Group A		crop rotation t <sub>cycle</sub> (yr	standard	Annual application rate ( input substance 1		custom			
Configure :	substance					stom calculation		-	<b>X</b>
custom		-		Help	K <sub>om</sub> (L/kg)	om/0.3			Help
Overall —			TIER 2b, 2c, and 3		7 Spatial par	rameters			Operators
Cod	de: custom substance 3			bymo	fraction of	organic matter (k	g/kg) [ om ]		+
K <sub>om</sub> (L/k	g): 31.0 K <sub>oc</sub> (L/kg): 5	.444	✓ use custom calculation	Set	pH (pH) [ p	h]			- *
DegT <sub>50</sub> (day	s): 14.0		use custom calculation	Set					
	pl): 300.0			501					log()
E (kJ/mo	bl):  65.4							A	dd Add
	0		Cancel			lent sorption			
	0		cancer		🔲 Use pH	dependent sorpti	on	K	(1.///a):
						рКа: Дрн:			, (L/kg): , (L/kg):
						црп.		om,a	
							Ok	Cancel	
							-		

Figure 44: Define custom calculation for K<sub>om</sub>

## 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'.

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Formula for pH dependent sorption:

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

pKa: negative logarithm of the dissociation constant

pH: pH correction factor

K<sub>OM, ba</sub>: organic matter/water distribution coefficient under basic conditions

K<sub>OM, ac</sub>: 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 Kom/DegT50:

- Calculated value for K<sub>om</sub> /DegT50 < Min value → use Min value</li>
  - Calculated value for K<sub>om</sub> /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 matte	r (kg/kg)	[om]	
рН (рН)		[ph]	

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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

custom	Help		
Overall Code: custom substance 2 K <sub>om</sub> (L/kg): 10.0 K <sub>oc</sub> (L/kg): 17.24 DegT <sub>50</sub> (days): 31.0	TIER 2b, 2c, and 3		
M (g/mol): 303.0 E (kJ/mol): 65.4	Configure substance	•	Help
Ok	Code: custom substance 2	TIER 2b, 2c, and 3	
	K <sub>om</sub> (L/kg): 10.0 K <sub>oc</sub> (L/kg): 17.24	use custom calculation	Set
	DegT <sub>50</sub> (days): 31.0 M (g/mol): 303.0	use custom calculation	Set

Figure 45: Delete a configured substance

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

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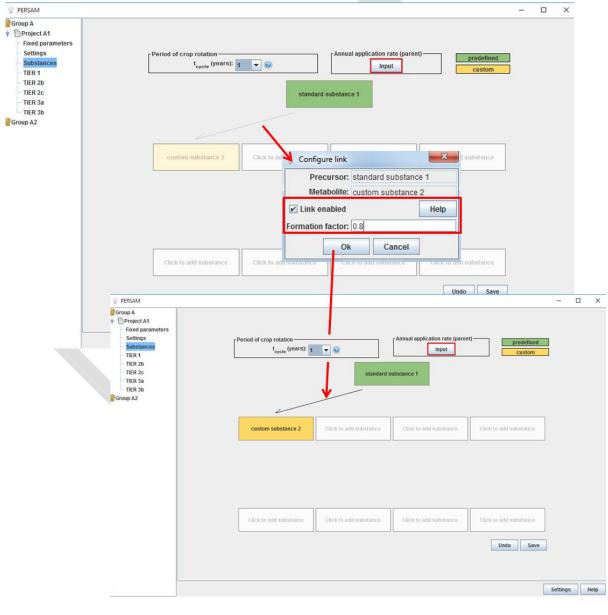
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# 7.6. Configure link

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

- 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'





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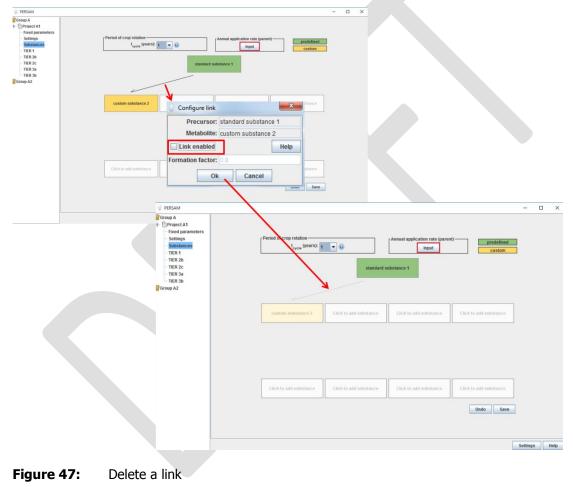


If a substance is configured where no arrows point to, this substance is removed when the user clicks the save button. This will also disable all arrows that start in that removed substance. If this renders additional substances into orphans (no arrows arrive there), then these substances are removed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



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# 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.

PERSAM								-		$\times$
Group A - Droject A1 - Fixed parameters - Settings	TIER 1 Overview Results									
- Substances TIER 1 TIER 2b TIER 2c TIER 2a										
TIER 3b Group A2		Zone(s) v north v centr south	al		oncentration in oncentration in					
		Parameters of	concentration	n in total soil-						
		Zone	T <sub>arit</sub> (K)	T <sub>arr</sub> (K)	$\theta_{fc} (m^3/m^3)$	ρ (kg/L)	f <sub>om</sub> (kg/kg)			
		north	277.85	280.15	0.244	0.95	0.118			
		central	281.15	283.25	0.244	1.05	0.086			
		south	284.15	285.45	0.385	1.22	0.048			
		Parameters of	concentration	n in liquid pha	se					
		Zone	T <sub>arit</sub> (K)	T <sub>arr</sub> (K)	$\theta_{fc} (m^3/m^3)$	ρ (kg/L)	f <sub>om</sub> (kg/kg)			
		north	281.35	282.95	0.347	1.39	0.023			
		central	282.25	284.35	0.347	1.43	0.018			
		south	285.95	287.85	0.347	1.51	0.011			
								Setting	s	Help

## 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:

- Zone(s) (see <u>settings section</u>)
- Endpoint(s) (see <u>settings section</u>)
- Substances (parent & metabolites) (see <u>substance section</u>)

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# 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  $f_{\rm M}$ .

## 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<sub>T,ini</sub>

	Symbol	Unit	Default values/Input
Parameter			
Initial total concentration in soil	C <sub>T,ini</sub>	mg.kg⁻¹	Formule [1]
Ecotoxicological averaging depth	Z <sub>eco</sub>	cm	1; 2.5; 5; 20 cm
Annual application rate	А	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:

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

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## Formula 4:

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

#### 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 <sup>-1</sup>	Formula 2
Ecotoxicological averaging depth	Z <sub>eco</sub>	cm	1; 2.5; 5; 20
Plough depth	Z <sub>til</sub>	cm	20
Initial total concentration in soil	C <sub>T,ini</sub>	mg.kg-1	Step 1
fraction of the dose left at the moment of the next application	X		Formula 3
Time between applications	t <sub>cycle</sub>	days	365; 730; 1095
Correction factor for temperature	f <sub>T</sub>		Formula 4
degradation rate coefficient at reference temperature	k <sub>ref</sub>	days⁻¹	Formula 5
Arrhenius activation energy	E	kJ.mol <sup>-1</sup>	Default 65.4; input field in Substances
Gas constant	R	kJ.mol <sup>-1</sup> .K <sup>-1</sup>	0.008314
Reference temperature	Tref	К	293.15
Arrhenius weighted average soil temperature	T <sub>arr</sub>	К	Corresponding to parameter T in formula 4
Half life for degradation in soil at 20°C	DegT50	days	Substance-specific parameter

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### Step 3: calculation of the maximum concentration in soil

#### Formula 6:

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

With:

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

	Symbol	U	Init	Default values/Input
Parameter				
Initial total concentration in soil	C <sub>T,ini</sub>	r	ng.kg <sup>-1</sup>	Step 1
Background concentration in soil just before next application	$C_{T,plateau}$	r	ng.kg-1	Step 2
Maximum total concentration in soil	$C_{T,peak}$	m	ng.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<sub>L,peak</sub>

	Symbol	Unit	Default values/Input
Parameter			
Maximum total concentration in soil	C <sub>T,peak</sub>	mg.kg⁻¹	Formula 3
Volumetric water content	$\theta_{\sf fc}$	m <sup>3</sup> .m <sup>-3</sup>	Soil-specific parameter
Dry bulk density	ρ	kg L⁻¹	Soil-specific parameter
Organic matter content	f <sub>omfc</sub>	kg.kg⁻¹	Soil-specific parameter
Organic matter/water distribution coefficient	K <sub>om</sub>	L.kg⁻¹	Substance-specific parameter
Maximum liquid concentration in soil	$C_{L,peak}$	mg.L⁻¹	Formula 7

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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:

	Symbol	Unit	Default values/Input
Parameter			
Time weighted average (TWA) total concentration in soil	C <sub>t,twa</sub>	mg.kg⁻¹	Formula 10
Maximum total concentration in soil	C <sub>T,peak</sub>	mg.kg⁻¹	Step 3
Time period since application time over which concentrations are averaged	t <sub>avg</sub>	days	7; 14; 21; 28; 56 days
Correction factor for temperature	f <sub>T</sub>		Formula 4
Degradation rate coefficient at reference temperature	k <sub>ref</sub>	days <sup>-1</sup>	Step 2
Maximum liquid concentration in soil	C <sub>L,peak</sub>	mg.L <sup>-1</sup>	Step 5
Time weighted average (TWA) liquid concentration in soil	C <sub>L,TWA</sub>	mg.L <sup>-1</sup>	Formula 10

## Step 6: calculation for metabolites

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

## Formula 13:

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

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### 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<sub>met,1</sub> and A<sub>met,2</sub>

	Symbol	Unit	Default values/Input
Parameter			
Formation fraction for the first metabolite	F <sub>f,1_p</sub>		Substance-specific parameter
Formation fraction for the second metabolite	F <sub>f,2_p</sub>		Substance-specific parameter
Molar mass of the first metabolite	M <sub>met,1</sub>	g.mol⁻¹	Substance-specific parameter
Molar mass of the second metabolite	M <sub>met,2</sub>	g.mol <sup>-1</sup>	Substance-specific parameter
Molar mass of the parent substance	M <sub>parent</sub>	g.mol⁻¹	Substance-specific parameter
Equivalent annual application rate first metabolite	A <sub>met,1</sub>	kg.ha <sup>-1</sup>	Formula 13
Annual application rate	А	kg.ha <sup>-1</sup>	Input field tab Substances
Equivalent annual application rate second metabolite	A <sub>met,2</sub>	kg.ha <sup>-1</sup>	Formula 14

# 8.2.2. Applying default scenario adjustment factor $\ensuremath{\,\,{\rm f}_{\rm s}}$ and model adjustment factor $\ensuremath{\,{\rm f}_{\rm M}}$

### Default scenario adjustment factors fs

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.

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C <sub>T,peak</sub> <sup>(a)</sup>	C <sub>L,peak</sub> (a)
3.0	2.0
2.0	1.5
2.0	1.5
	3.0 2.0

#### Table 11: Default scenario adjustment factors f<sub>s</sub> for PERSAM crops

(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)

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# 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 or	n the zone and	d endpoint

		Symbol				Unit				
Parameter										
Temperature	T <sub>Arit</sub>	T <sub>Arit</sub>				К				
Temperature	T <sub>Arr</sub>	T <sub>Arr</sub>				к				
Volumetric wa	ater content	-				m <sup>3</sup> m <sup>-3</sup>				
Dry bulk dens	ity				Kg L⁻¹					
Organic matter content		f <sub>om</sub>				kg.kg <sup>-1</sup>				
				-						
PERSAM									- 0	
Group A	TIER 1									
Project A1 Fixed parameters	Overview Results									
TIER 2c TIER 3a TIER 3b Group A2		Zone(s)	rat		oncentration in oncentration in					
		r Parameters	concentration	in total soil						
		Zone	T <sub>arit</sub> (K)	Т <sub>ант</sub> (К)	$\theta_{fc} (m^3/m^3)$	p (kg/L)	f <sub>om</sub> (kg/kg)			
		north	277.85	280.15	0.244	0.95	0.118			
		central	281.15	283.25	0.244	1.05	0.086			
		south	284.15	285.45	0.385	1.22	0.048			
		Parameters	concentration				1			
		Zone	T <sub>arit</sub> (K)	T <sub>arr</sub> (K)	$\theta_{f_0}$ (m <sup>3</sup> /m <sup>3</sup> )	p (kg/L)	fom (kg/kg)			
		north	281.35	282.95	0.347	1.39	0.023			
		central	282.25 285.95	284.35 287.85	0.347	1.43	0.018			
		south	280.90	287.85	0.347	1.91	0.011			



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## 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.

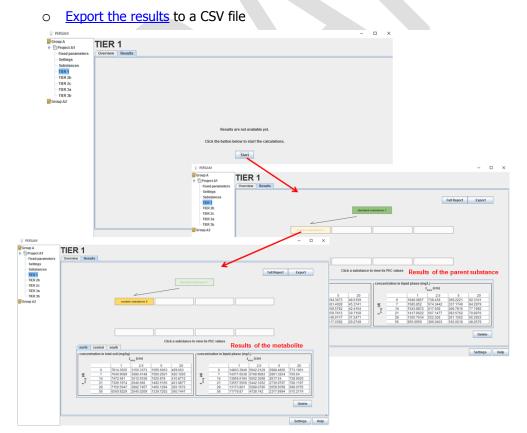
Calcu	ation in progress, please wait	
	Cancel	

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:**

- Delete the results
- <u>Create a PDF report</u> of the results



### Figure 51: Results of TIER-1

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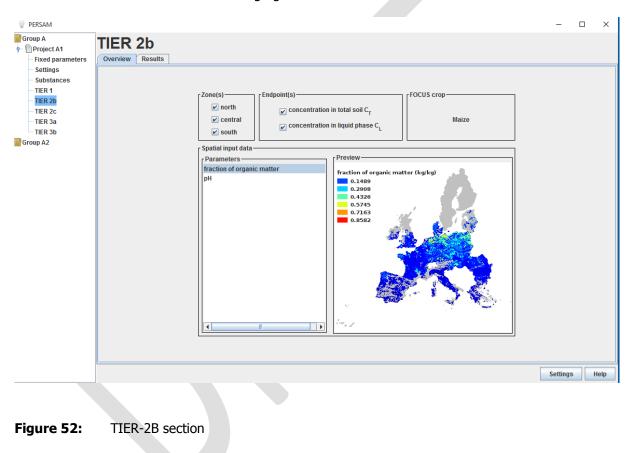
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# 9. TIER-2B

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



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

## 9.1. TIER-2B settings

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

- Zone(s) (see <u>settings section</u>)
- Endpoint(s) (see <u>settings section</u>)
- FOCUS crop (see <u>settings section</u>)
- Substances (parent & metabolites) (see <u>substance section</u>)

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

# 9.2. TIER-2B calculations

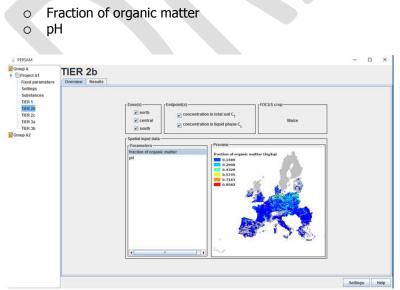
The calculation for the 95the spatial percentile of the PEC with the simple analytical model is as follows:

- ✓ 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<sub>L,peak</sub> or C<sub>T,peak</sub> or any of the TWA averages) for the required ecotoxicological averaging depth (z<sub>eco</sub>) and for the DegT50 K<sub>om</sub> properties of this substance.
- ✓ Calculate from this concentration map the cumulative frequency distribution of PEC values. In this calculation the PEC of each 1x1km<sup>2</sup> pixel should get a weight that is proportional of the fraction of surface area grown with this crop or crop group.
- $\checkmark$  Take the 95<sup>th</sup> 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:





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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.

💡 PERSAM		-		×
♥ PERSAM         Group A         ♥ Troject A1         ■ Frixed parameters         Substances         ■ TER 2b         ■ TER 2b         ■ TER 2b         ■ TER 3a         ■ Group A2         ● Project A2.1         ■ Fixed parameters         ■ Substances         ■ TER 3b         ■ Group A2         ● Project A2.1         ■ Fixed parameters         ■ Substances         ■ TER 2b         ■ TER 3a         ■ TER 3b         ● Project A2.2	Zone(s)       Endpoint(s)         Image: concentration in total soil Cr       Spring Cereals (not further specifil)         Spatial input data       Parameters         Image: real specific concentration of organic matter (kg/kg)       Free vertice (kg/kg)         Image: real specific concentration of organic matter (kg/kg)       Image: real specific concentration of organic matter (kg/kg)	-		×
	Concentration in total soll			
		Setting	3	Help

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

### **Other functionalities:**

• Delete the results

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• <u>Create a PDF report</u> of the results



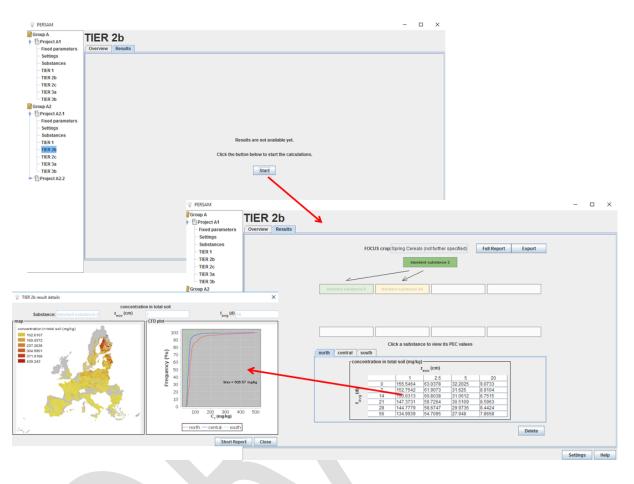


Figure 55: Results of TIER-2B

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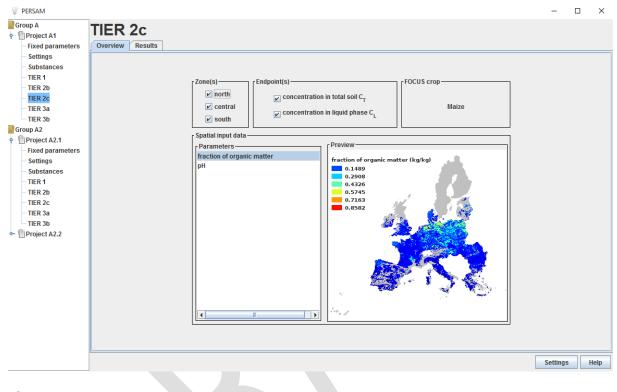
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# 10. TIER-2C

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:

- Zone(s) (see <u>settings section</u>)
- Endpoint(s) (see <u>settings section</u>)
- FOCUS crop (see <u>settings section</u>)
- Substances (parent & metabolites) (see <u>substance section</u>)
- 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 <u>Configure custom</u> <u>calculations</u>)

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## **10.2. TIER-2C calculations**

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

The calculations of TIER-2C are based on the calculations of TIER-2B (see TIER-2B calculations)

The relationship between TIER-2B and TIER-2C is following formula:

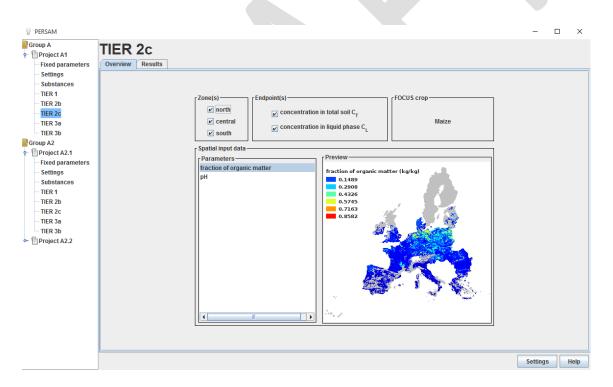
PEC  $_{2C} = F_{soil,max} PEC_{2B}$ 

# 10.3. TIER-2C overview

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

The spatial input maps are:

- Fraction of organic matter
- 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.

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Therefore the overview window of TIER-2C presents different spatial input data.

PERSAM		-		×
Group A Project A1 Fixed parameters Settings	TIER 2c Overview Results			
- Substances - TIER 1 - TIER 2b - TIER 2c - TIER 3a - TIER 3b	Zone(s)			
Group A2 ↑ Droject A2.1 Fixed parameters - Settings - Substances - TIER 1 - TIER 26 - TIER 3a - TIER 3a	Spatial input data  Parameters  Iraction of organic matter (kg/kg)  Ph  Concentration in total soil  Concentration in total soil  T  T  T  T  T  T  T  T  T  T  T  T  T			
		Setting	s	Help

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.
- Click on a cell in the table to view extended results. A detail window appears containing the 95<sup>th</sup> spatial percentile of calculated PECs for the regulatory selected zone with the related cumulative distribution graph and map

### Other functionalities:

- Delete the results
- <u>Create a PDF report</u> of the results
- Export the results to a CSV file

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# 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.

PERSAM		-		$\times$	
Group A	Zone(s)       Endpoint(s)         Image:	-		×	
=	With: <i>f<sub>z</sub></i> default scenario adjustment factor <i>f<sub>z</sub></i> default at Tier-2A <i>PEC</i> <sub>Tier-2A</sub> ; PEC predicted at Tier-2A				
		Settings	ŀ	Help	

Figure 59: TIER-3A section

## 11.1. TIER-3A settings

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

- Zone(s) (see <u>settings section</u>)
- Endpoint(s) (see <u>settings section</u>)
- FOCUS crop (see settings section)
- Substances (parent & metabolites) (see <u>substance section</u>)

## **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 <sub>Tier-3A</sub> =	$\frac{Result_{Tier-2B}}{Result_{Tier-1}/f_s}REC_{Tier-2A}$

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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.

## 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:

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

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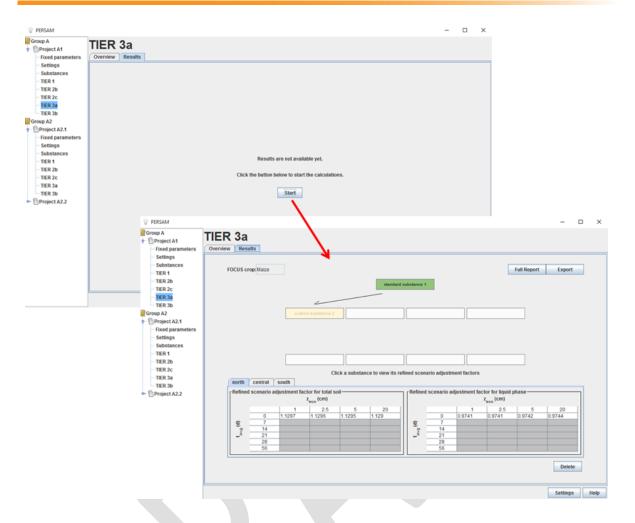


Figure 61: TIER-3A results tab

# 12. TIER-3B

TIER-3 is designed to select the grid cell including the scenario properties corresponding to the 95<sup>th</sup>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.

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PERSAM		_		×
Group A	TIER 3b			
Fixed parameters	Overview Results			
Settings Substances TIER 1 TIER 2c TIER 2c TIER 3a Frier 3b Group A2 Fixed parameters Substances TIER 1 TIER 2b TIER 2c TIER 1 TIER 2b Substances TIER 1 TIER 3a TIER 3a TIER 3a	Zone(s)       Image: Concentration in total soil C <sub>T</sub> FOCUS crop         Image: Concentration in total soil C <sub>T</sub> Image: Concentration in total soil C <sub>T</sub> Maize         Image: Concentration in liquid phase C <sub>L</sub> South       Maize			
	Parameters fraction of organic matter pH Preview fraction of organic matter (kg/kg) 0.1489 0.2908 0.3226 0.3745 0.8582 0			
		Setti	ngs	Help

Figure 62: TIER-3B section

# 12.1. TIER-3B settings

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

- Zone(s) (see <u>settings section</u>)
- Endpoint(s) (see <u>settings section</u>)
- FOCUS crop (see <u>settings section</u>)
- Substances (parent & metabolites) (see <u>substance section</u>)

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# **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 95<sup>th</sup> 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:

- Fraction of organic matter
- o pH

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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.

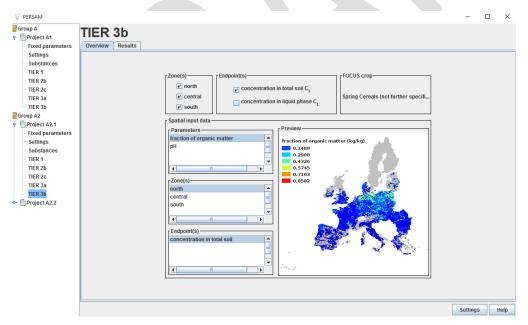


Figure 64: TIER-3B overview tab for FOCUS crop 'Spring Cereals(not further specified)'

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# **12.4. TIER-3B results**

The user can start the calculations and view the results.

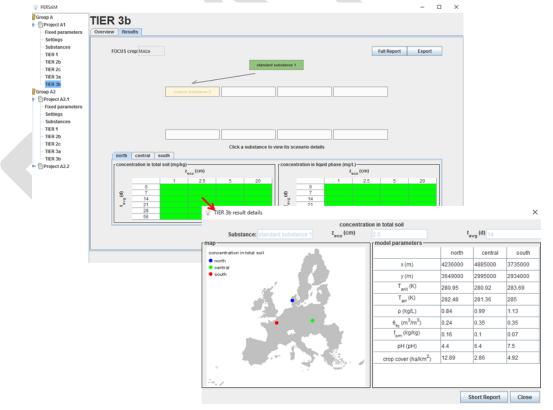
- 1. Go to the 'Results' tab
- 2. Select a substance in the Substance tree to view the results. The results tab of TIER-3 contains a table with the green cells which indicates whether there results are available.
- 3. Click on a particular cell (a combination of ecotoxicological averaging depth, time 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:**

- Delete the results
- <u>Create a PDF report</u> 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.





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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.

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# **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.

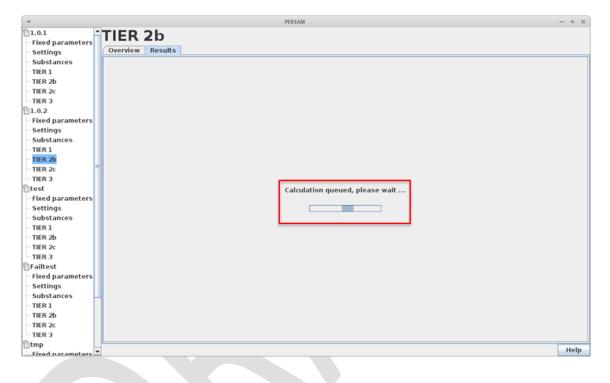


Figure 66: Batch processing – calculations are still running

# 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.

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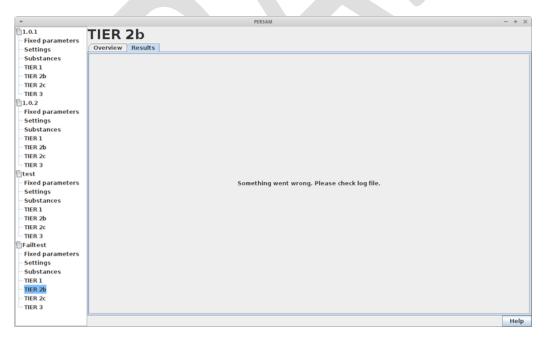
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- TIER 2b - TIER 2c - TIER 3 ⊡Failtest	Undo Save	
Fixed parameters     Settings     Substances     TIER 1     TIER 2b     TIER 2c     TIER 3		

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

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# 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:

-	Batch processing
	Ongoing calculations. Are you sure you to exit PERSAM?
	Yes

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:

*	Unsaved changes X		
	Changes were made in the current vi Are you sure you to exit PERSAM?	ew.	
	Yes No		

# 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:

•	Existing calculations
?	Do you want to continue processing the existing batch queue or do you want to empty it
	Continue Empty
_	

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'.

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# 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

PERSAM		- 0	×
Group A   Group A    Fixed parameters  Fixed parameters  Fixed parameters  Group A2	Time between applications t <sub>cycle</sub> (prears): 1 • • • • • • • • • • • • • • • • • •		
	Click to add substance Click to add substance Click to add substance Undo 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'

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- 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.

**<u>Remark</u>**: 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.

roup A quor	IER 1	
Projectiva		
	verview Results	
- Settings		
Substances		Full Report Export
TIER 1		
TIER 2b	standard substance 1	
TIER 2c		
TIER 3a		
TIER 3b	Generate report	
roup A2	summer substance 2	
Project A2.1	Save In: 🕀 Local Disk (C:)	- 6 - 8 -
Fixed parameters		
Settings	drivers 🖸 Users	
Substances	intel VITO	
TIER 1	PerfLogs 🔂 Windows	
TIER 2b	Program Files	
TIER 2c	Program Files (x86)	
TIER 3a	north central south	
TIER 3b	TEMP	
Project A2.2	concentration in total soil (mg/kg)	
	Z <sub>eco</sub> (CM)	
	1 2.5 File Name: Project A1.1 - TIER 1 report.	
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# 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  $T_{avg}$ 

**<u>Remark</u>**: 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.





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# **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.

PERSAM						$\times$
Group A	TIER 3b					
- Fixed parameters	Overview Results					
<ul> <li>Settings</li> <li>Substances</li> <li>TIER 1</li> <li>TIER 2b</li> </ul>	FOCUS crop:Maize			Full Report	Export	
- TIER 2c - TIER 3a	💡 Export		standard substance 1			
TIER 3b Group A2	Look In:	] Documents	■ a a a 85			
Project A2.1     Fixed parameters     Settings     Substances     TIER 1     TIER 2b     TIER 2c     TIER 3a     TIER 3b	north central					
Project A2.2	concentration in t File Name:	Project A1 - TIER 3b.csv		(mg/L)		
	Files of <u>Type</u>	e: CSV files (*.csv)	<b>•</b>	z <sub>eco</sub> (cm)		
	(c) (c) (c) (c) (c) (c) (c) (c)		Export Cancel	2.5 5	20	
					Delete	
_					Settings	Help
Figure 72:	Exporting results					

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#### **Additional information** 15.

This section contains additional information such as:

- FOCUS Crops 0
- **EFSA Spatial version** 0

#### 15.1. **FOCUS Crops**

Next table contains the FOCUS crop list.

## Table 13: FOCUS crops

FOCUS crop	PERSAM crop	CTN	СТС	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 <sup>(a)</sup>	JO	CH	KR	HA	CH	TH
Peas (animals)	Pulses	JO	CH	-	HA	CH	-
Potatoes <sup>(b)</sup>	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
	Barley	JO	CH	KR	HA	CH	PO
	Common wheat	JO	CH	KR	HA	CH	PO
Spring cereals <sup>(c)</sup>	Durum wheat	-	CH	KR	-	CH	PO
	Oats	JO	CH	KR	HA	CH	PO
	Rye	JO	CH	KR	HA	CH	PO
	Barley	JO	CH	KR	HA	CH	SE
	Common wheat	JO	CH	KR	HA	CH	SE
Winter cereals(c)	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.

(a): Not a POCUS crop; therefore, onions are suggested as a surrogate in the numerical models at lefs 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. 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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# 15.2. EFSA Spatial data

The EFSA spatial data set version 1.1 includes following maps:

Table 14: EFSA Spatial data version 1	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

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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

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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 <u>http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/</u>

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# **16.** Troubleshooting and Helpdesk

Troubleshooting during the installation procedure:

# • There is not enough disk space:

The software requires 1.2GB disk space for the installation.

It is advisable to provide 10 GB of free disk space to comfortably work with PERSAM for the sake of the required temporary disk space

## • User rights:

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

# Problem reporting:

## Following information is required for reporting the problem.

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

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

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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

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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



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# **Abbreviations**

CAPRI	Common Agricultural Policy Regionalised Impact model
CL	Liquid concentration in soil (mg.L <sup>-1</sup> )
C <sub>T</sub>	Total concentration in soil (mg.kg <sup>-1</sup> )
DegT <sub>50</sub>	Degradation half-life in soil (days)
ρ	Dry bulk density of the soil (kg.dm <sup>-3</sup> )
E	Arrhenius activation energy
f <sub>M</sub>	Model adjustment factors
f <sub>om</sub>	Organic matter content (-)
f <sub>s</sub>	Default scenario adjustment factors
f <sub>soil</sub>	Fraction that reaches the soil (-)
K <sub>om</sub>	Organic matter/water distribution coefficient (L.kg <sup>-1</sup> )
М	Molar mass
R	Gas constant
T <sub>arit</sub>	Arithmetic mean temperature (K)
T <sub>arr</sub>	Arrhenius weighted average soil temperature (K)
t <sub>avg</sub>	Averaging time
t <sub>cycle</sub>	Time between applications
T <sub>ref</sub>	Reference temperature
$\theta_{\text{fc}}$	Water content at field capacity $(m^3.m^{-3})$
Z <sub>eco</sub>	Ecotoxicological averaging depth
Z <sub>til</sub>	Plough depth

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# Appendix A – FOCUS Crops<sup>1</sup>

FOCUS crop	PERSAM crop	CTN	СТС	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	ОК
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 <sup>(a)</sup>	JO	CH	KR	HA	CH	TH
Peas (animals)	Pulses	JO	CH	-	HA	CH	_
Potatoes <sup>(b)</sup>	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
	Barley	JO	CH	KR	HA	CH	PO
	Common wheat	JO	CH	KR	HA	CH	PO
Spring cereals <sup>(c)</sup>	Durum wheat	-	CH	KR	-	CH	PO
	Oats	JO	CH	KR	HA	CH	PO
	Rye	JO	CH	KR	HA	CH	PO
	Barley	JO	CH	KR	HA	CH	SE
	Common wheat	JO	CH	KR	HA	CH	SE
Winter cereals(c)	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.

<sup>1</sup> 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

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# Appendix B – Soil-specific parameters<sup>2</sup>

## 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 <sub>arit</sub> <sup>(a)</sup> (°C)	Т <sub>ат</sub> <sup>(b)</sup> (°С)	Texture	$f_{om}(-)^{(c)}$	$\theta_{fc} (\mathrm{m}^3 \mathrm{m}^{-3})^{(\mathrm{d})}$	ρ (kg dm <sup>-3</sup> ) <sup>(e)</sup>
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): Tarit is the arithmetic mean annual temperature

(b): Tarr is the Arrhenius-weighted mean annual temperature (explained in EFSA PPR Panel, 2012a)

(c): fom (-) is the organic matter content

(d):  $\theta_{fc}$  (m<sup>3</sup> m<sup>-3</sup>) is the water content at field capacity

(e): ρ (kg dm<sup>3</sup>) 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 <sub>arit</sub> <sup>(a)</sup> (°C)	Т <sub>ат</sub> <sup>(b)</sup> (°С)	Texture	$f_{om} \left( - \right)^{(c)}$	$\theta_{fc} (\mathrm{m^3 \ m^{-3}})^{(d)}$	ρ (kg dm <sup>-3</sup> ) <sup>(e)</sup>
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): Tarit is the arithmetic mean annual temperature

(b): Tarr is the Arthenius-weighted mean annual temperature (explained in EFSA PPR Panel, 2012a)

(c): f<sub>om</sub> (-) is the organic matter content

(d):  $\theta_{fc}$  (m<sup>3</sup> m<sup>-3</sup>) is the water content at field capacity

(e): ρ (kg dm<sup>-3</sup>) 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.

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<sup>&</sup>lt;sup>2</sup> 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 C – Substance - specific parameters<sup>3</sup>

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

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

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<sup>&</sup>lt;sup>3</sup> 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