EXTERNAL SCIENTIFIC REPORT

APPROVED: 18 February 2021

doi:10.2903/sp.efsa.2021.EN-1756

Update of PERSAM software models for predicting environmental concentrations in soil in permanent crops and annual crops:

User manual PERSAM 3.0.5

VITO NV

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

Abstract

PERSAM is a software tool for predicting environmental concentrations of plant protection products (PPPs) in soil commissioned by EFSA. The PERSAM tool was first launched in 2013. In support of the EFSA Guidance Document for predicting environmental concentrations of PPPs in soil (2017), the PERSAM software tool was updated for calculating the predicted environment concentration of PPPs in soil. The computerized tools will be released for use by applicants and risk assessors for the evaluation of PPPs and transformation products according to Parliament and Council Regulation (EC) 1107/2009. The software application assists the user in performing calculations using the analytical model, as described in the guidance document for predicting environmental concentrations of PPPs in soil (2017). More specifically, the software will be able to calculate Tier-1 Predicted Environmental concentrations, Tier-2 95th-percentile PECs and selection of the grid cell including the scenario properties corresponding to the 95th-percentile PEC as needed for the scenario development at Tier 3A and generation of a so-called transfer file that can be read by the numerical models described in the Guidance Document. PERSAM generates reports intended for regulatory submissions. Based on these reports the authorities need to be able to check or reproduce the model results. This report contains the user manual of the PERSAM version 3.0.5.

Key words: Exposure assessment, soil, plant protection products, metabolites, soil organisms, tiered approaches, crop interception

Question number: EFSA-Q-2017-00563

Correspondence: pesticides.ppr@efsa.europa.eu

Suggested citation: VITO NV, 2021. Update of PERSAM software models for predicting environmental concentrations in soil in permanent crops and annual crops. EFSA supporting publication 2021:EN-1756. 96 pp. doi:10.2903/sp.efsa.2021.EN-1756

ISSN: 2397-8325

Summary

In EFSA, the Pesticides Units (PREV and PRES) and the Panel on Plant Protection Products and their Residues (PPR) are responsible for activities related to 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 EFSA PRAPeR Unit noted that the existing SANCO Guidance Document (SANCO/9188VI/1997 of 12 July 2000) needs to be updated.

VITO developed the PERSAM tool, a software tool for predicting environmental concentrations of plant protection products (PPPs) in soil commissioned by EFSA. The PERSAM tool was first launched in 2013. In support of the EFSA Guidance Document for predicting environmental concentrations of PPPs in soil (2017), the PERSAM software tool was updated for calculating the predicted environment concentration of PPPs in soil.

The software application assists the user in performing calculations using the analytical model, as described in the guidance document for predicting environmental concentrations of PPPs in soil (2017). More specifically, the software will be able to calculate:

- ✓ Tier-1 Predicted Environmental concentrations,
- ✓ Tier-2 95th-percentile PECs
- ✓ Selection of the grid cell including the scenario properties corresponding to the 95th-percentile PEC as needed for the scenario development at Tier 3A and generation of a so-called transfer file that can be read by the numerical models described in the Guidance Document.

PERSAM generates reports intended for regulatory submissions. Based on these reports the authorities need to be able to check or reproduce the model results.

The user manual includes the description of input screens and the Tier-1 and Tier-2 calculations of the PERSAM v3.0.5.

Table of contents

User manual PERSAM 3.0.5 1
VITO NV 1
Abstract 1
Summary 3
1. Introduction 6
1.1. Background and Terms of Reference as provided by the requestor 6
1.2. What's new? 6
1.2.1. PERSAM v3.0.0 6
1.2.2. PERSAM v3.0.1 8
1.2.3. PERSAM v3.0.2 8
1.2.4. PERSAM v3.0.3 8
1.2.5. PERSAM v3.0.4 9
1.2.6. PERSAM v3.0.5 9
2. Installation 9
2.1. System requirements 9
2.2. Standard installation 10
2.3. Maps 12
2.4. Licensing 13
2.5. Version number 13
3. Project management 13
3.1. Group 14
3.1.1. New group 14
3.1.2. Rename group 15
3.1.3. Delete group 16
3.2. Project 16
3.2.1. New project 17
3.2.2. Rename project 18
3.2.3. Change project output folder 19
3.2.4. Duplicate project 19
3.2.5. Delete project 20
3.2.6. Import project 20
3.2.7. Export project 21
3.2.8. Document management 22
4. Wizard 25
4.1. Wizard: start screen 25
4.2. Wizard: Selection of region type 27
4.3. Wizard: Selection of zone(s) 27
4.4. Wizard: Selection of EU country 28
4.5. Wizard: Selection of crop type 28
4.6. Wizard: Selection of endpoint(s) 28
4.7. Wizard: Selection of Focus crop 29
4.8. Wizard: Selection of application type 30
5. Settings 30
5.1. Tier-1: Settings 30
5.2. Tier-2 & Tier-3A: Settings 31
5.3. Change settings 32
5.3.1. Change zone and application type 32
5.3.2. Change crop and endpoint 34
6. Substances 36
6.1. Configure predefined substance 37
6.2. Configure custom substance 38
6.3. Delete a substance 38

6.4. Configure link 39
6.5. Delete a link 40
6.6. Configure custom calculations 41
7. Application scheme 43
8. Fixed data 44
8.1. Tier-1: Fixed data 44
8.1. Tier-2 & Tier-3A: Fixed data 45
9. Calculations 46
9.1. Tier-1: Calculations 47
9.2. Tier-2: Calculations 51
9.3. Tier-3A: Calculations 58
10. Results 59
10.1. Tier-1: Results 59
10.2. Tier-2 & Tier-3A: Results 59
11. Report management 62
11.1. Advanced reports 62
11.2. Short report 63
12. Batch processing 64
12.1. Batch mode 64
12.2. Import multiple projects 64
13. Additional information 66
13.1. Crop Interception Factors 67
13.2. Crop specification list 73
13.3. EFSA Spatial data 74
13.4. FOCUS Crops 77
13.5. f_{ridge} and f_{furrow} for spray applications 79
13.6. f_q, $f_{om,corr}$, z_{til}, $C_{T,ini}$ and $C_{T,plateau}$ in relation to crop and application type 79
13.7. Scenario and model adjustment factors 81
13.8. Soil specific parameters 83
13.9. Wash-off fractions of the dose intercepted by Crop canopy 84
13.10. Overview PERSAM input parameters 89
13.11. PERSAM 3 export/import file format 90
13.11.1. JSON 90
13.11.2. Valid export files 90
13.11.3. High level export file structure 90
13.11.4. Project fields 91
13.11.5. The properties object 91
13.11.6. The settings object 92
13.11.7. The substanceTree object 92
13.11.8. The applicationScheme object 94
References 95
Abbreviations 96

1. Introduction

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

In EFSA, the Pesticides Units (PREV and PRES) and the Panel on Plant Protection Products and their Residues (PPR) are responsible for activities related to 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 EFSA PRAPeR Unit noted that the existing SANCO Guidance Document (SANCO/9188VI/1997 of 12 July 2000) needs to be updated.

VITO developed the PERSAM tool, a software tool for predicting environmental concentrations of plant protection products (PPPs) in soil commissioned by EFSA. The PERSAM tool was first launched in 2013. In support of the EFSA Guidance Document for predicting environmental concentrations of PPPs in soil (2017), the PERSAM software tool was updated for calculating the predicted environment concentration of PPPs in soil.

The computerized tools will be released for use by applicants and risk assessors for the evaluation of PPPs and transformation products according to Parliament and Council Regulation (EC) 1107/2009.

This contract was awarded by EFSA to:

Contractor: VITO NV
Contract: "Update of PERSAM software models for predicting environmental concentrations of plant protection products in soil in permanent crops and annual crops
Contract number: OC/EFSA/PRAS/2018/01

1.2. What's new?

1.2.1. PERSAM v3.0.0

New features of PERSAM v3.0.0 are:

- ✓ Wizard for guiding the user when starting a new project
- ✓ New input parameters:

	New input parameters
Tier- 1	Crop type (annual/permanent)
	Microbial active substance
	Time interval for calculation of post-application PEC

Tier-2	Crop type
	Microbial active substance incl. crop interception
	Time interval for calculation of post-application PEC
	Type of application
	Incorporation/soil depth z_{inc}
	Fraction of surface area treated $f_{treated}$
	RAC value, total soil
	RAC value, pore water

- ✓ Scenario and adjustment factors are visible in the tool at the section of fixed parameters.
- ✓ The tool should alert the user when a parameter is out-of-range or has not been entered.
- ✓ All temperatures must be entered in the unit °C.
- ✓ The software tool provides the option that the user can reset the analysis options to system defaults.
- ✓ The user can select a zone or an EU country
- ✓ At Tier-1 and Tier-2, the user shall be able to select one eco-toxicological evaluation depth z_{eco} for concentration in total soil and/or concentration in pore water, and one time weighted average t_{avg}. The PERSAM tool shall calculate two results, one result based on the default values, and one result based on the user-specific parameters.
- ✓ The software tool shall contain the latest version, available at the JRC website, of spatial data, including e.g. new maps for permanent crops, a map with EU Member States, … .
- ✓ PERSAM should contain updated pH-maps so that red colours is displaying acid soils and blue colours basic soils.
- ✓ The short reports and the advanced reports include all scenario properties, calculated results, the peak concentration, the plateau concentration, and if applicable also the fraction of area treated or incorporation depth. The reports are intended for regulatory submissions. Based on these reports the authorities need to able to check or reproduce the model results.
- ✓ Scenario and adjustment factors are visible in the tool at the section of fixed parameters.
- ✓ The x-scale at the results of Tier-2 are limited to e.g. 2 times the 95th percentile of the worst-case zone.
- ✓ The pH-map is included in the report when a pH-dependent substance is simulated
- ✓ PERSAM contains updated pH-maps so that red colours is displaying acid soils and blue colours basic soils.
- ✓ The tool allows to select TWA's up to 100 days.
- ✓ The software tool provides the option that the user can reset the analysis options to system defaults.

- ✓ The legend of the Tier-2 maps are chosen according to an equal percentile classification where each percentile range has an equal area. Colours of the maps are always be chosen so that the highest values have reddish colours and the lowest values have greenish colours.
- ✓ Tier-3A does not require additional model inputs but the algorithm must avoid extreme scenario properties
- ✓ The user can import a JSON file and start the calculations in batch mode
- ✓ Tier-2 and Tier-3A are combined in one project
- ✓ PERSAM generates a transfer file for PEARL and PELMO

1.2.2. PERSAM v3.0.1

Issues solved in PERSAM v3.0.1 are:

- ✓ Adaption of the Tier-3 calculation:

  In case only a limited number of cells contain the crop for which the assessment is carried out, it can be that not all percentile intervals contain cells. According to the calculation procedure, for the Tier-3A scenario selection the cells between the 94th and 96th (area weighted) percentile must be used. If for example the crop coverage is 4 cells, it can be that cell 1 is the 10th percentile, cell 2 the 34th percentile, cell 3 the 68th percentile and cell 4 the 100th percentile. In this case, the 94-96 percentile interval is completely between cell 3 and cell 4. PERSAM will then select the cell just above the interval to build the Tier-3A scenario, which is cell 4 in the example.

- ✓ Importing several projects with one JSON file

1.2.3. PERSAM v3.0.2

New features in PERSAM v3.0.2 are:

- ✓ Update to Java 11 (fixes some UI hiccups)
- ✓ If the crop is not present in the selected zone/county, the new project wizards displays a warning message
- ✓ A zip file containing the spatial data in ARC/INFO ASCII grid format is included in the distribution
- ✓ Substance codes can no longer contain invalid characters for filenames (list of invalid characters extended to "*")
- ✓ Bug fix: for microbial active substances the DT50 value is no longer reset to the default once it is overridden

1.2.4. PERSAM v3.0.3

New features in PERSAM v3.0.3 are:

- ✓ the no-crop-present warning message is also shown when the crop is not present in a subset of the selected regions (previously only if not present in all of the selected regions) and the message also lists the regions where the crop is not present

1.2.5. PERSAM v3.0.4

New features in PERSAM v3.0.4 are:

- ✓ Bug fix: problems with the installer when installing the software in a location where a previous installation (using an older Java version) was present. In PERSAM 3.0.4 this is solved in the installer and the issue does not occur anymore.

1.2.6. PERSAM v3.0.5

New features in PERSAM v3.0.5 are:

- ✓ Bug fix: problems with the installer when installing in a folder with a pathname containing spaces. In PERSAM 3.0.5 this is solved in the installer and the issue does not occur anymore.
- ✓ The no-crop-present warning message is revised: when the crop is not present in one or more of the selected regions the message is given "Crop is not present in this (all of these) zone(s)/countr(y)(ies) of evaluation: []. Please select a different crop or zone/country." and the user cannot proceed with the calculation

2. Installation

Installation of the PERSAM requires no additional licensed software tools or applications. The software is down-loadable and will automatically be installed on your pc.

For more information go to the JRC soil portal (*http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/)* The software requires 1.2GB disk space for the installation. It is advisable to provide 10 GB of free disk space to comfortably work with PERSAM for the sake of the required temporary disk space.

Recommendations before starting the installation

- Install the PERSAM software with the user rights of the user who will use the PERSAM tool
- The default installation folder is the 'user' folder. It is important to use a folder where the user has write rights and the folder size can increase to 1 GB.

Installation of PERSAM

First the user should agree to the license agreement before PERSAM can be installed via a standard installation (UI installation)

2.1. 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 11.0.8_10 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.

2.2. Standard installation

Installation procedure

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

2. Download the software:

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

   or

   → Start immediately the installation

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

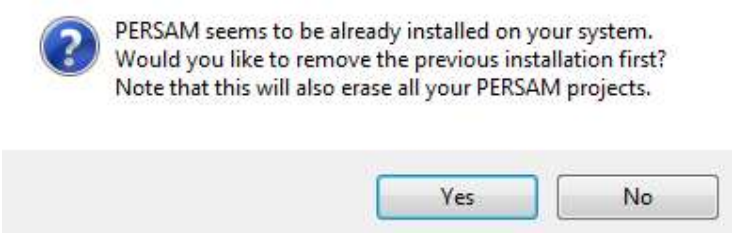


Figure 1: Message 'PERSAM already installed'

   → Yes: all PERSAM projects will be erased

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

4. Starting the installation procedure

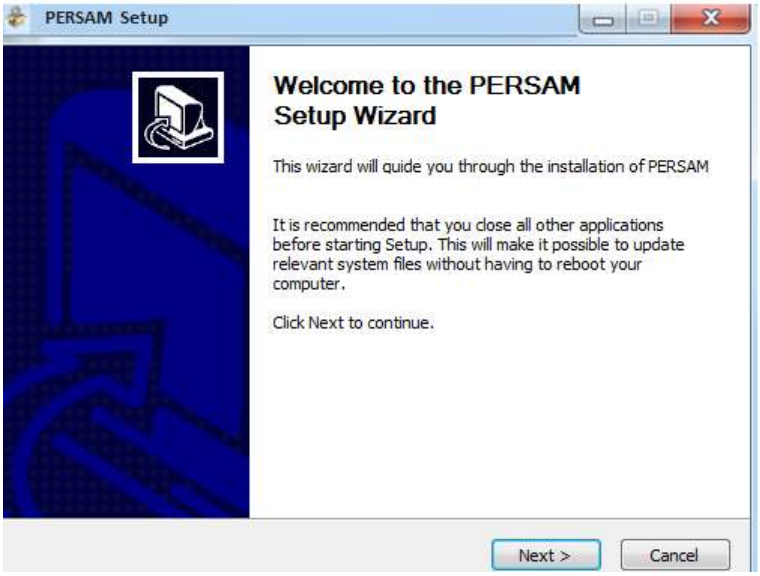


Figure 2: Installation procedure – Welcome screen

→ Click on 'Next'

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

→ Choose the installation directory:

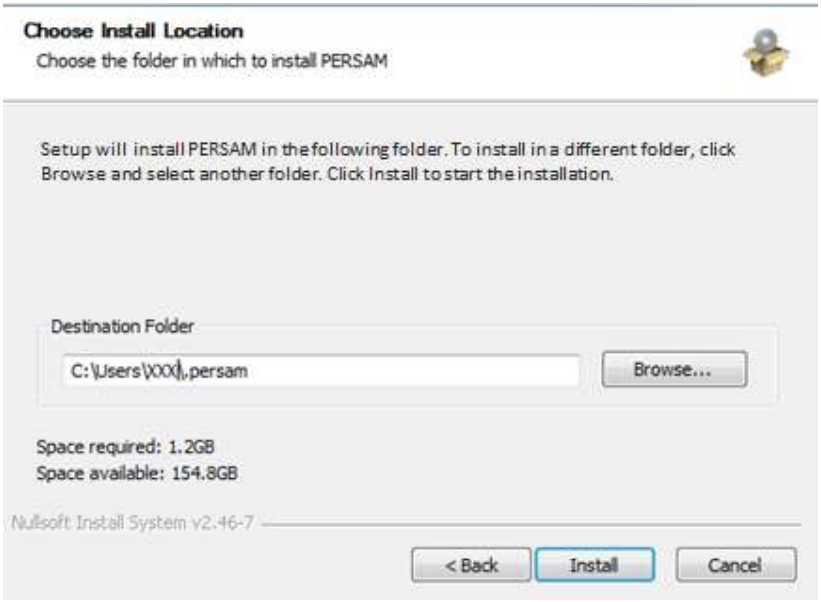


Figure 3: Installation procedure – Choose installation directory

→ Select the destination folder and click on 'Install'

→ The installation will start

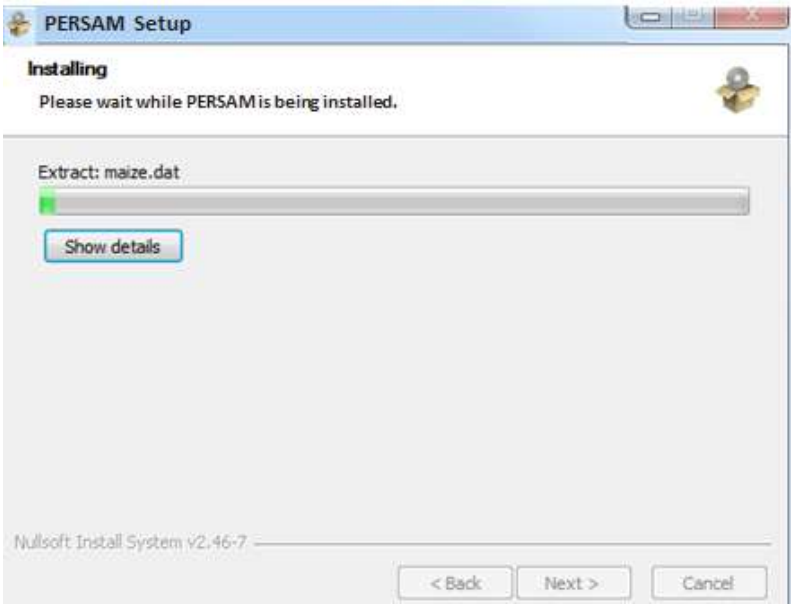


Figure 4: Installation procedure – Installing the software

→ After the installation, click on 'Finish'

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

Figure 5: PERSAM application in start menu

2.3. Maps

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

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

2.4. Licensing

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

2.5. Version number

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

Current PERSAM version number (incl. revision number): v3.0.2-

Figure 6: Where can you find the current version number of PERSAM?

3. Project management

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

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

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

- Project operations:
  - Define a new project:
    - an empty project
    - from a previously exported project (import a project)
    - from a duplicated project
  - Open an existing project
  - Duplicate a project
  - Export a project:
  - Delete a project

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

Figure 7: Project management tree

3.1. Group

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

Related functionalities:

- New group
- Rename group
- Delete group

3.1.1. New group

The user creates a new group.

1. Right mouse click in the left pane of the Welcome window and select 'New group' or click on the 'New group …' button
2. Give a group name
3. Click on 'Create group'

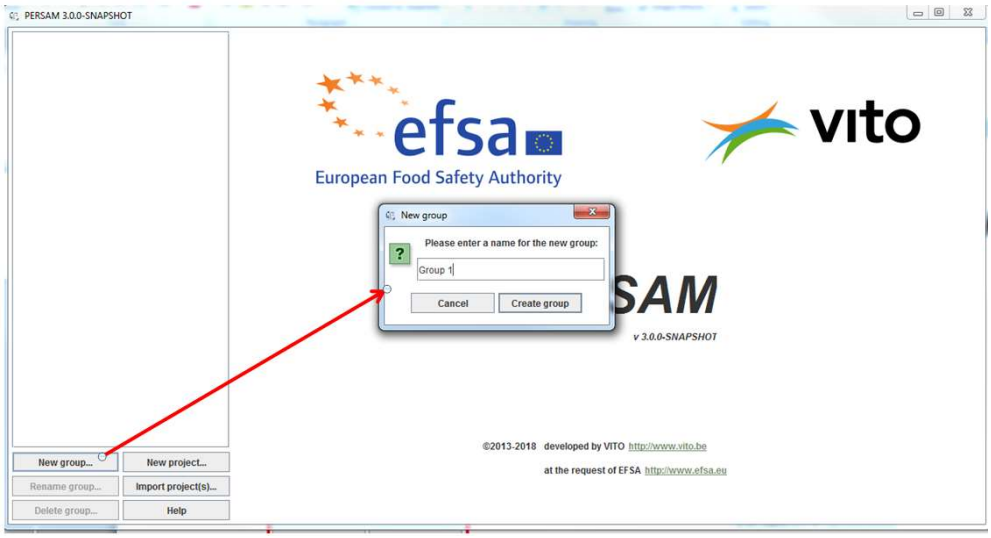


Figure 8: New group

3.1.2. Rename group

The user can give another name to an existing group.

1. Select a group
2. Right mouse click and select 'Rename group' or click on the 'Rename group' button.
3. Give a new name
4. Click on 'Rename group'

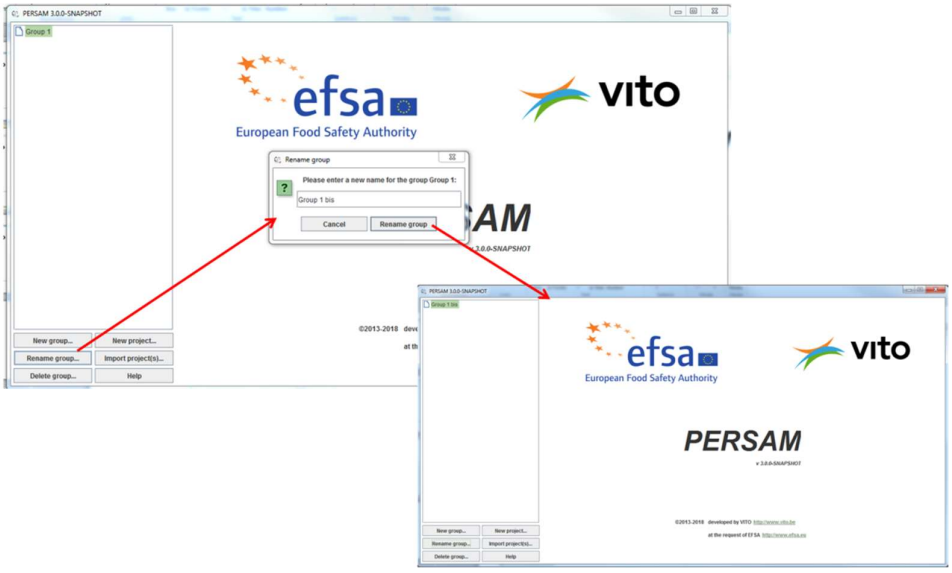


Figure 9: Rename group

3.1.3. 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' or click on the 'Delete group' button
3. Following message appears: *Delete the following group and all its contents?*
   - ✓ Delete group: delete the selected group
   - ✓ Cancel: don't delete the selected group

Figure 10: Project management – Delete a group

3.2. 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: Settings, Substances, Application scheme, Fixed data and Results.

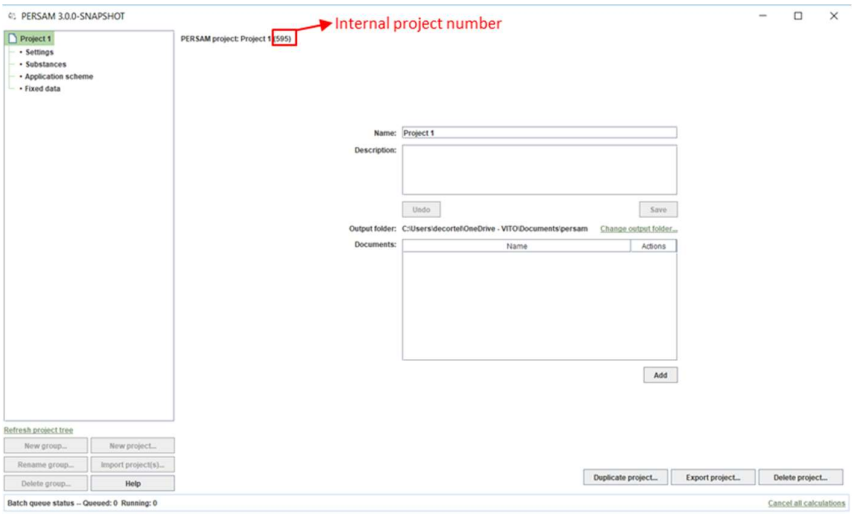


Figure 11: Project main screen

The number next to the project name is an internal unique PERSAM number for a project.

The projects are sorted in alphabetic order in the projects tree.

Documents

The user can add relevant documents to the project.

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

Related project functionalities:

- New project
- Rename project
- Change project output folder
- Duplicate project
- Delete project
- Import project
- Export project

3.2.1. New project

The user creates a new project by clicking on the 'New project' button or right mouse click and select 'New project'. The user is guided through a wizard where he defines several parameters before PERSAM creates the project. The wizard process is described in detail in section 5.

When PERSAM creates a project, the project is added to the project panes, left on the screen. Every project contains the same structure that compromises the settings, substances, application scheme, fixed data and results.

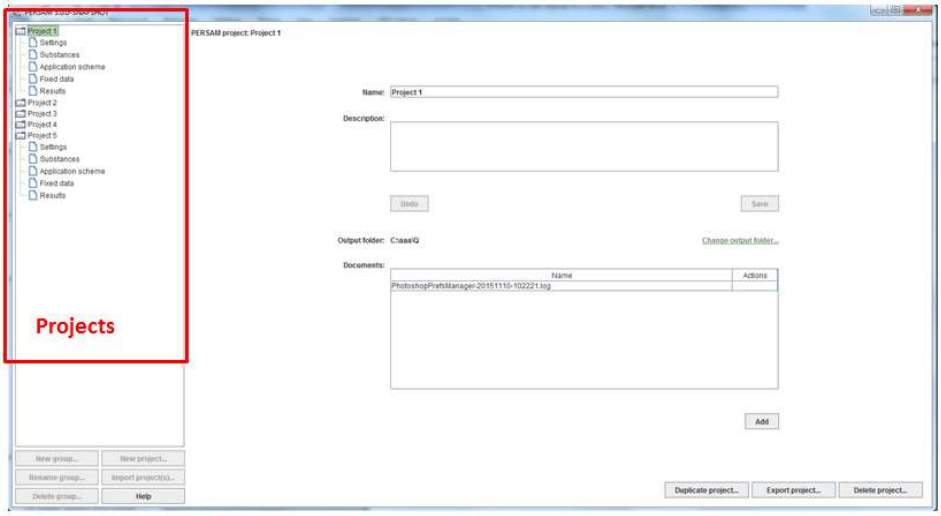


Figure 12: Projects

3.2.2. Rename project

The user changes the project name of an existing project.

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

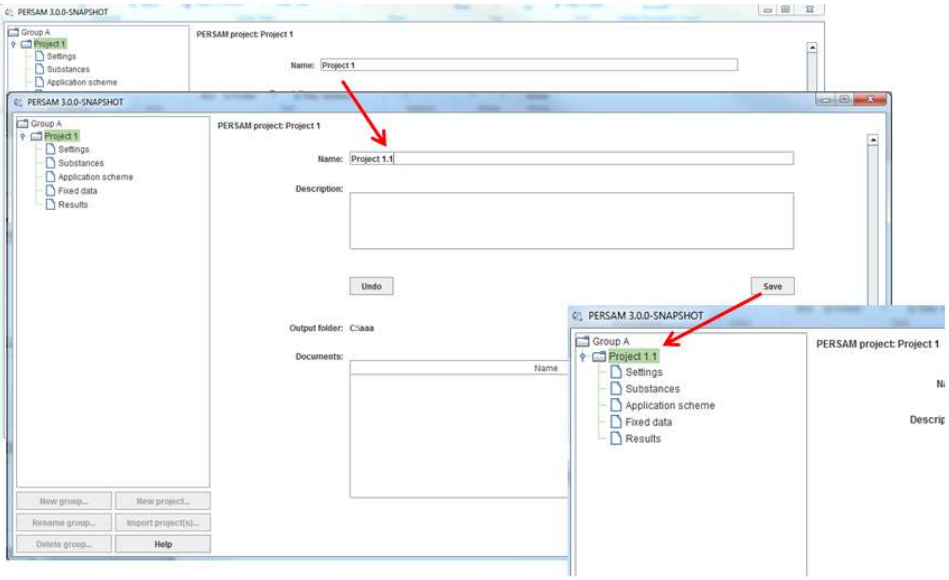


Figure 13: Rename project

3.2.3. Change project output folder

The user changes the project output folder.

1. Select an existing project
2. Go to the project window
3. Click on 'Change output folder …', next to the output folder.
4. A popup windows appears for selecting a new folder
5. Click on 'Save'

3.2.4. Duplicate project

The user can duplicate an existing project.

1. Select a project
2. Right mouse click and select 'Duplicate project'
3. Give the new name for the project and click on 'OK'
4. The new project is added to the project tree.

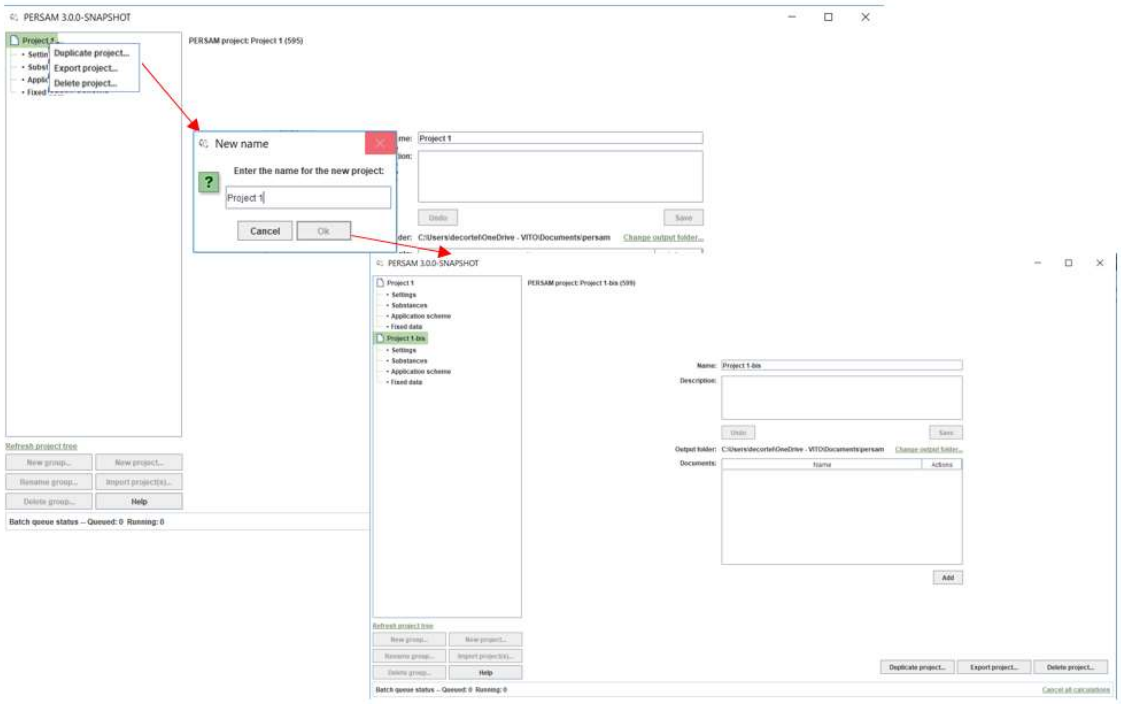


Figure 14: Duplicate project

3.2.5. Delete project

The user can delete an existing project.

1. Select a project
2. Right mouse click and select 'Delete project' or click on the 'Delete project' button at the bottom of the project screen
3. Following message appears: *Delete project XXX?*
   - Delete project: delete the selected project
   - Cancel: don't delete the selected project

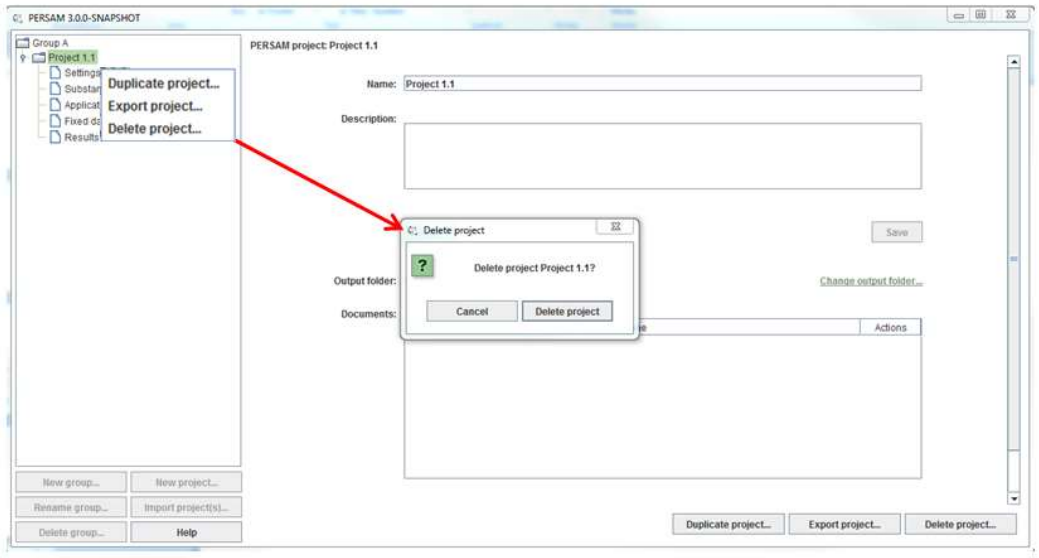


Figure 15: Project management – Delete project

3.2.6. Import project

The user can import an existing project.

1. Click on the with space in the projects tree
2. Right mouse click and select 'Import project(s)' or click on the 'Import project(s)' button at the bottom of the project screen
3. Select the project(s) that you want to import and click on 'Open'
4. A message appears for starting the calculations
   - Yes: The calculations are scheduled in the batch queue
   - No: The calculations are not scheduled in the batch queue

- Cancel: The import of project(s) is cancelled.

The import files are in JSON format. More info see section 13.11 PERSAM 3 export/import file format.

Figure 16: Project management – Import project

3.2.7. Export project

The user can export an existing project.

1. Select a project
2. Right mouse click and select 'Export project'
3. Select the folder for the export file
4. Enter a file name and click on the 'Save' button

The export files are in JSON format. More info see section 13.11 PERSAM 3 export/import file format.

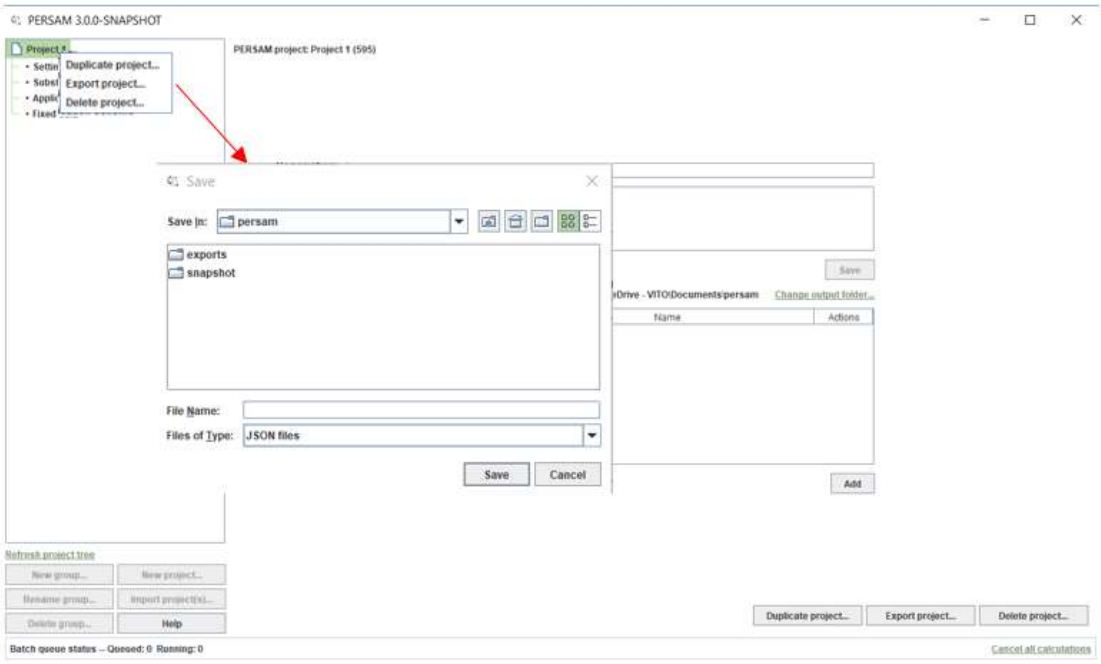


Figure 17: Project management – Export project

3.2.8. Document management

The user can add relevant documents to the project.

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

Next document types are supported:

- Excel
- Word
- PDF
- TXT
- CSV

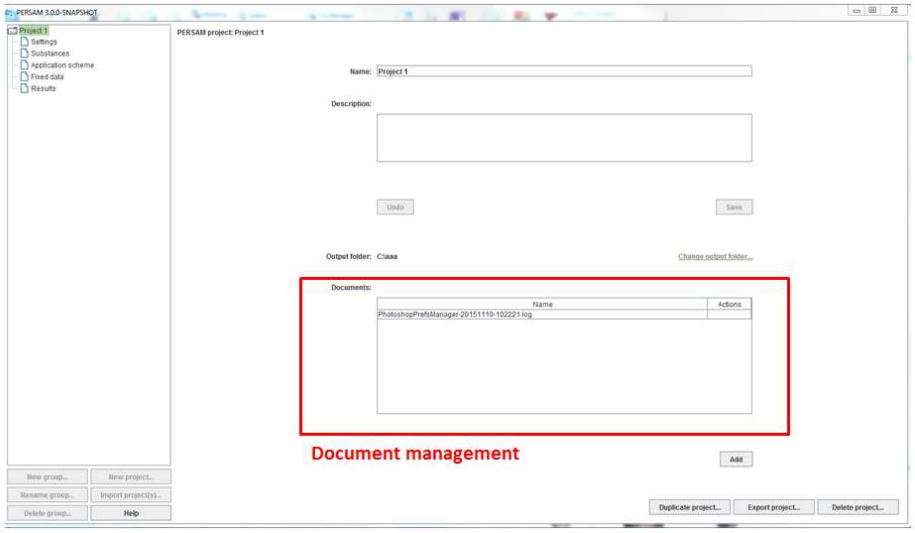


Figure 18: Project – Document management

Add document

The user can add a relevant document to the project.

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

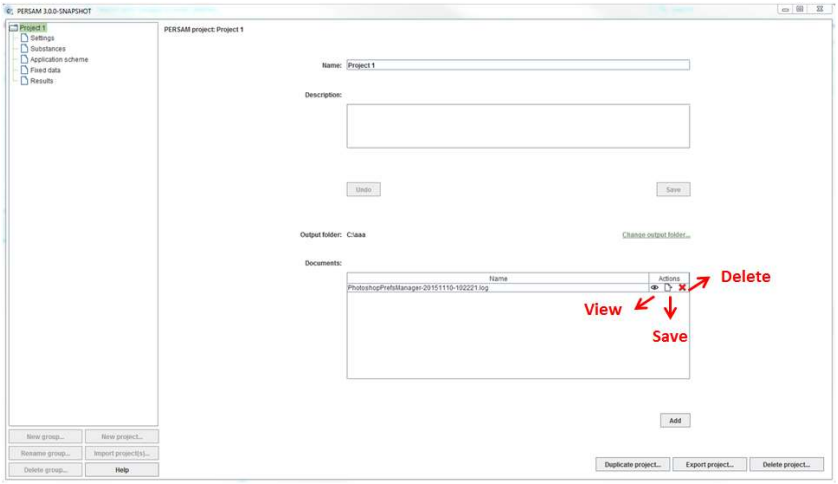


Figure 19: Project – Document actions

When a document is added to the project, it appears in the overview. Other document actions are view document, save document and delete document.

View document

The user can view the documents related to the project.

1. Point with your cursor to a particular document and the document actions are visible.
2. Click on the view icon and the document will be opened.

The user can only consult excel files, word documents, pdf documents, txt files and csv files.

Save document

The user can export documents related to the project.

1. Point with your cursor to a particular document and the document actions are visible.
2. Click on the save icon
3. There appears a popup window where you define the export name and the location for the export file .
4. Click on 'Save'

Delete document

The user can delete a document related to the project.

1. Point with your cursor to a particular document and the document actions are visible.
2. Click on the delete icon
3. Following message appears: *Delete document [document name]?*
   - Delete document: delete the selected document
   - Cancel: don't delete the selected document

4. Wizard

When starting a new project the wizard guides you through different steps where you have to define the parameters. Finally PERSAM creates a project based on the settings of the wizard. The figure below gives an overview of the wizard process.

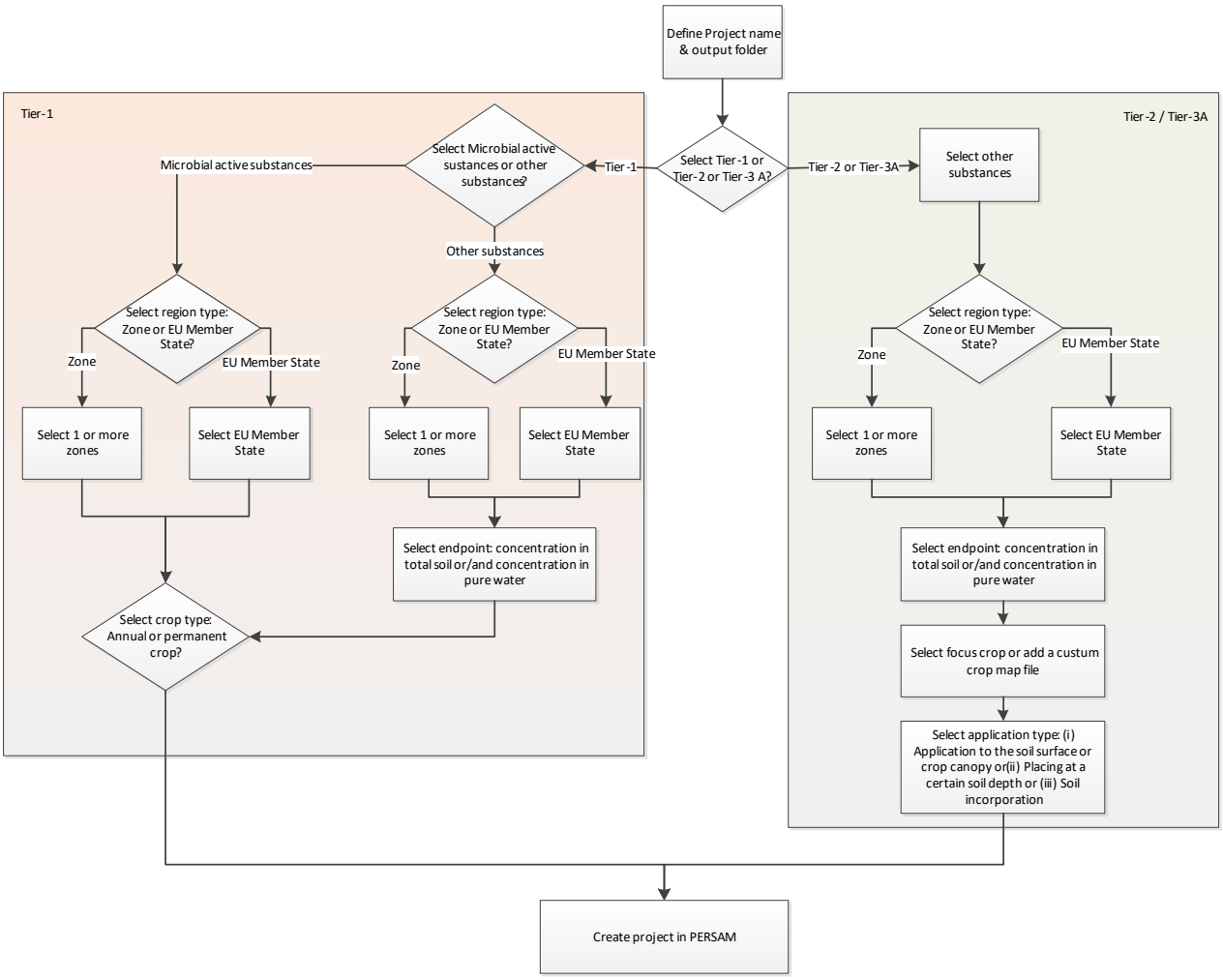


Figure 20: Wizard process

4.1. Wizard: start screen

In start screen you need to define a project name, the output folder and select the Tier and type of substances.

1. Enter the project name (required)
2. Select an output folder where PERSAM stores the generated output files (reports, output file for numeric models, …) of the project.(required)
3. Select Tier-1 or Tier-2 & Tier-3A by clicking on the tier:
    - **TIER-1** consists of calculations for six scenarios: three regulatory zones North, Centre, South and two endpoints in soil, i.e. concentration in pore water and total

concentration in soil. The scenarios apply to both annual and permanent crops. The user selects one or more scenarios (North, Centre, South) with its associated input parameters, a crop type (permanent or annual crop) and one or two endpoints (pore water concentration, total concentration in soil). The application calculates the PEC values for the selected parameters.

- **Tier-2** is based on a spatially-distributed version of the analytical model and is used to calculate the 95th-percentile PECs for the intended use area in each regulatory zone. 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 is present. The procedure differs for irrigated and non-irrigated crops. In non-irrigation crops precipitation, organic matter and temperature refer to the location of each individual pixel. In the case of irrigated crops, however, precipitation and irrigation are lumped together and are constant throughout the entire regulatory zone. The respective amount of precipitation + irrigation to be used for irrigated crops is specified by the mean annual precipitation of the dominant crop. In this tier, relationships between K_{om} and DegT50 and soil properties can be incorporated in the calculations. The output is the statistical distribution of concentrations for the considered endpoint and averaging depth from which the overall 95th percentile can be selected. In Tier-2, it suffices to calculate the 95th spatial percentile of the PEC of the required type of concentration.

- At **Tier-3A**, the tool should give the 95th-percentile scenario location for the parent as well as each metabolite together with all scenario and substance properties. PERSAM generates specific scenarios for each type of concentration, for each regulatory zone and for each evaluation depth for both, parent and metabolites. The scenarios selection is done in a way that extreme scenario properties are avoided.

Remark: Tier-2 and Tier-3A are always selected together.

4. Select the substances type. Microbial actives substances are only available for Tier-1.

5. Click on 'Next'

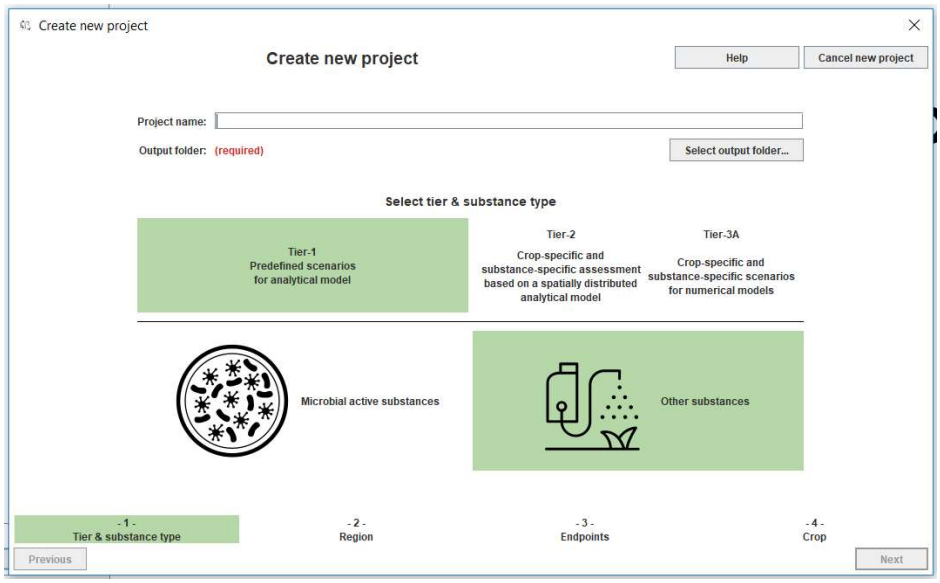


Figure 21: Wizard: Start screen

4.2. Wizard: Selection of region type

1. Select the region type by clicking on Zone(s) or on EU Country

   Remark: This selection is only available for Tier-2 & Tier-3A. Tier-1 works only with zones.

2. Click on 'Next'

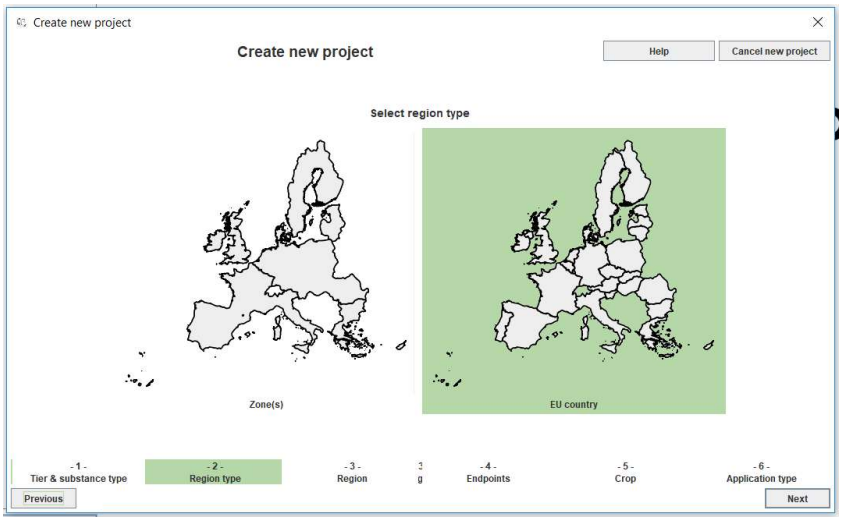


Figure 22: Wizard: Selection of region type

4.3. Wizard: Selection of zone(s)

1. Select one of more zones on the map by clicking on the zone(s) or select the zone(s) in the list. Select multiples zones in the list by using control button or select the whole list by using the shift button.

2. Click on 'Next'

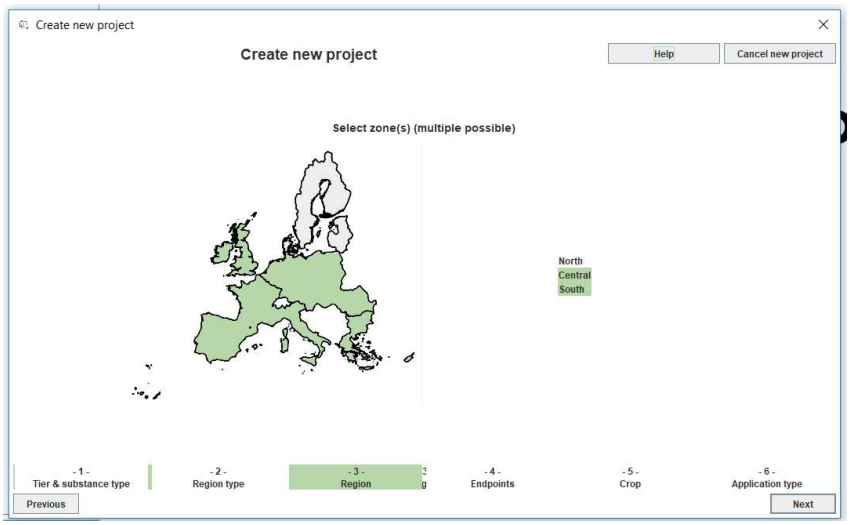


Figure 23: Wizard: Selection of zone(s)

4.4. Wizard: Selection of EU country

1. Select an EU country on the map or select one from the list. You can also give the first characters and the list goes automatically to the related country.
2. Click on 'Next'

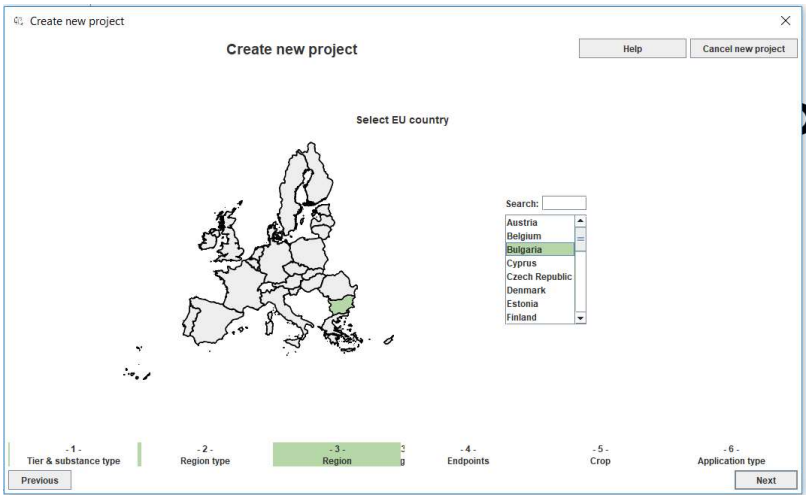


Figure 24: Wizard: Selection of EU country

4.5. Wizard: Selection of crop type

1. Select one crop type by clicking on 'Annual crop' or 'Permanent crop'.
2. Click on 'Next'

Figure 25: Wizard: Selection of crop type

4.6. Wizard: Selection of endpoint(s)

1. Select one or more endpoints by clicking on 'Concentration in total soil C_T' and/or 'Concentration in pore water C_L'.

2. Click on 'Next'

Figure 26: Wizard: Selection of endpoint(s)

4.7. Wizard: Selection of Focus crop

1. Select a Focus crop from the list or upload your custom crop map file. The format of the crop map file is an ASCII grid file.. In the list you can give the first characters and the list goes automatically to the related Focus Crops.
2. Click on 'Next'

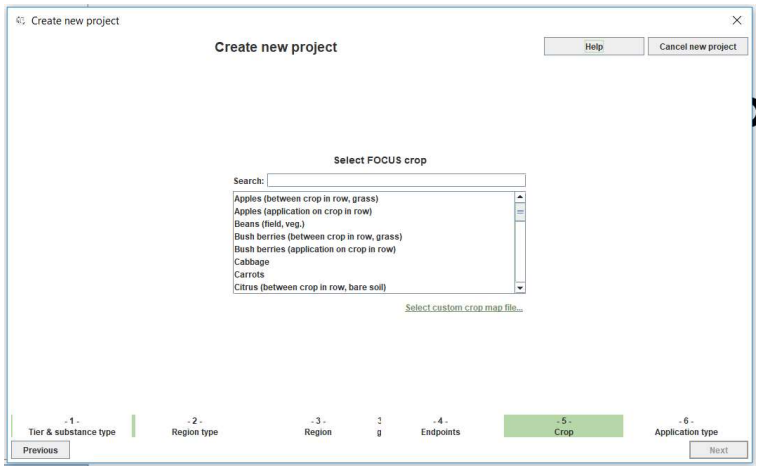


Figure 27: Wizard: Selection of Focus crop

If the crop is not present in (one of) the zone(s)/country for which the evaluation is carried out, a warning will be given: "Crop is not present in all of these zones/countries of evaluation: []. Please select a different crop or zone/country." and the user cannot proceed with the calculation.

If the user wants to evaluate application to bare soil, for permanent crops bare soil between rows should be selected and for annual crops an early growth stage of the following crop.

4.8. Wizard: Selection of application type

1. Select one application type by clicking on 'Application to the soil surface' or 'Application to the crop canopy' or 'Placing at a certain soil depth' or 'Soil incorporation'.
2. Click on 'Next'

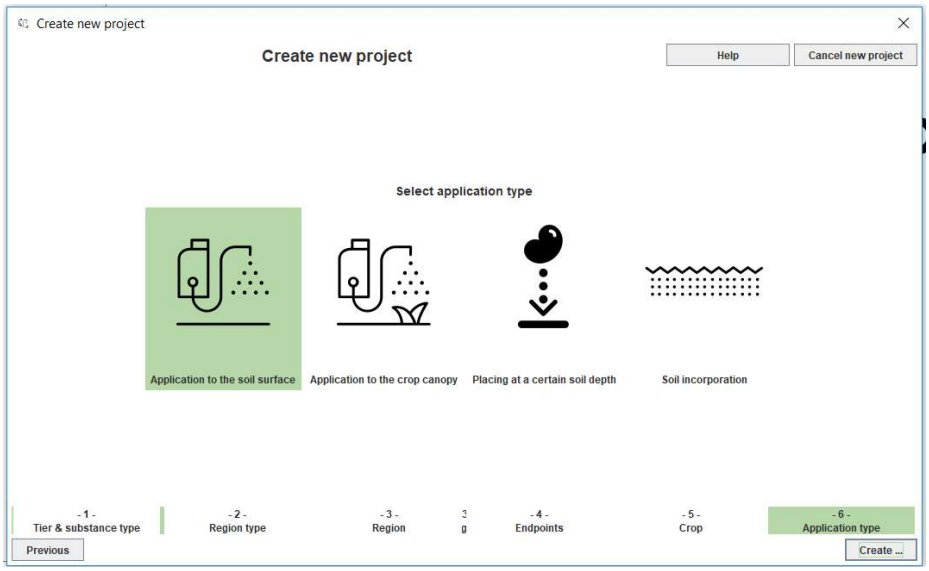


Figure 28: Wizard: Selection of Application type

5. Settings

The settings screens contain the project properties, defined in the wizard. The project properties are dependent on the selected tier.

5.1. Tier-1: Settings

The project properties are the defined parameters of the wizard. The Tier-1 settings for the calculation of the PEC values are described in the table below.

Table 1: Project settings for Tier-1

Parameter	Description
t_{avg}	Time weighted average t_{avg} in days. The default value is 0 days
$t_{Post/app}$	Time interval for calculation of post-application PEC in days. The default value is 0 days. This parameter is part of the PERSAM transfer file.
Z_{eco} (total soil)	Eco-toxicological evaluation depth Zeco for concentration in total soil C_T (by default: 5cm) on the condition that concentration in total soil is selected.
Z_{eco} (pore water)	Eco-toxicological evaluation depth Zeco for concentration in liquid phase C_L (by default: 1cm) on the condition that concentration in pore water is selected. If microbial active substance is selected in the wizard, Zeco for C_L is disabled

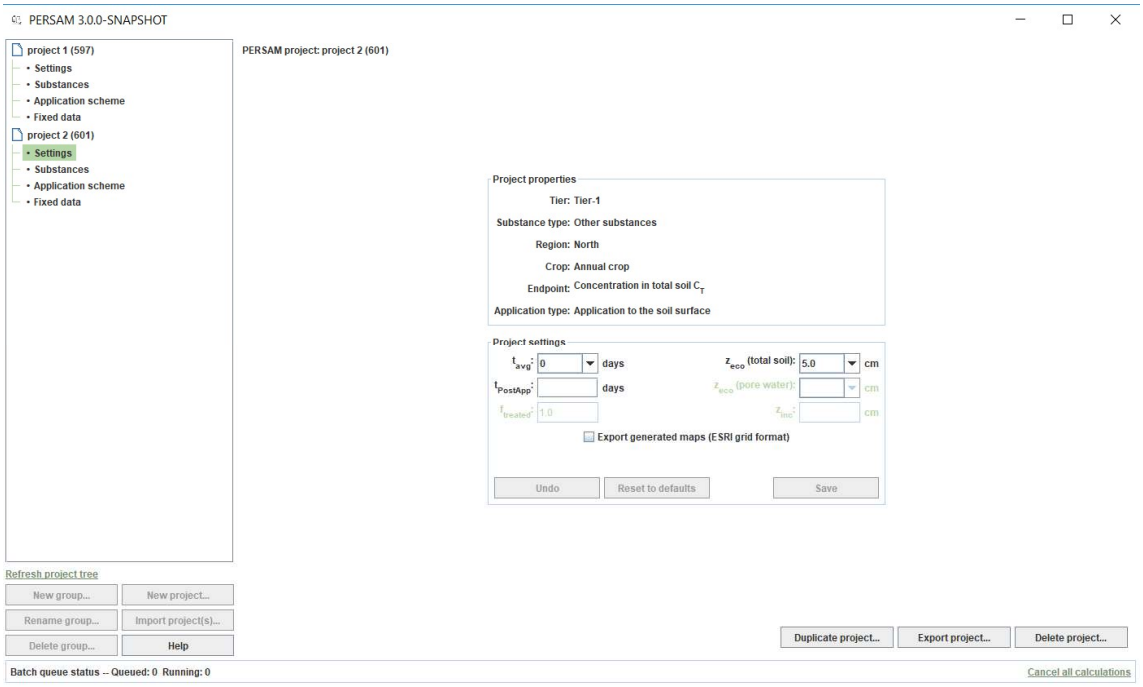


Figure 29: Tier-1 settings

5.2. Tier-2 & Tier-3A: Settings

The project properties are the defined parameters of the wizard. The Tier-2 and Tier-3A settings for the calculation of the PEC values are described in the table below.

Table 2: Project settings for Tier-2 and Tier-3A

Parameter	Description
t_{avg}	Time weighted average t_{avg} in days. The default value is 0 days
$t_{Post/app}$	Time interval for calculation of post-application PEC in days. The default value is 0 days. This parameter is part of the PERSAM transfer file.
Z_{eco} (total soil)	Ecotoxicological evaluation depth Zeco for concentration in total soil C_T (by default: 5cm) on the condition that concentration in total soil is selected.
Z_{eco} (pore water)	Ecotoxicological evaluation depth Zeco for concentration in liquid phase C_L (by default: 1cm) on the condition that concentration in pore water is selected. If microbial active substance is selected in the wizard, Zeco for C_L is disabled
z_{inc}	The incorporation/soil depth z_{inc} in cm is disabled when the type application is 'Application to the soil surface or crop canopy'. The values of z_{inc} depends on the application type. When the application type is 'Placing at a certain soil depth', the valid values are from 0 to 29 cm. When the type of application is 'Soil incorporation' the valid values for annual crops are from 1 to 30 cm and for permanent crops the valid values are 1,5,10,20 and 30. The default value is 0.
$f_{treated}$	The fraction of surface area treated $f_{treated}$ is disabled and fixed at the default 1.0 for permanent crops. For annual crops $f_{treated}$ is user input.

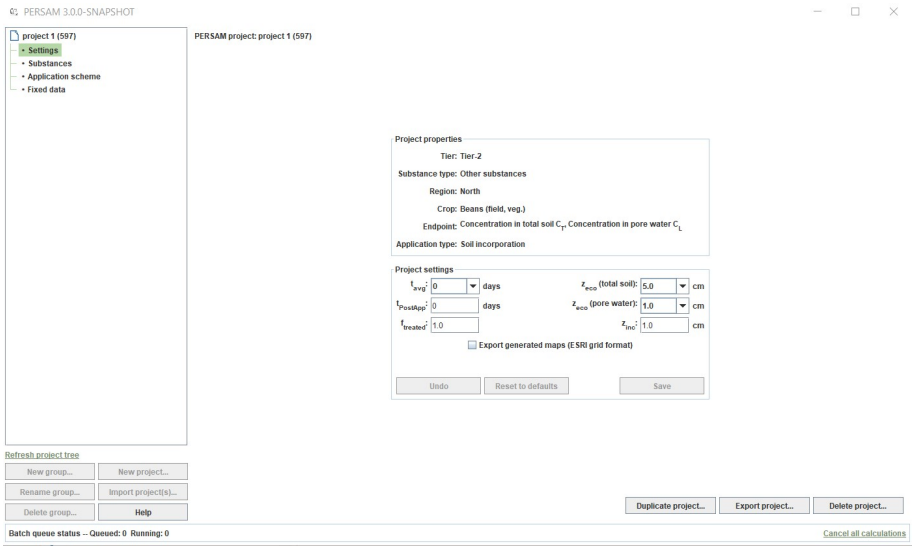


Figure 30: Tier-2: Settings

5.3. Change settings

The project properties are the defined parameters of the wizard and cannot be changed in the settings screen.

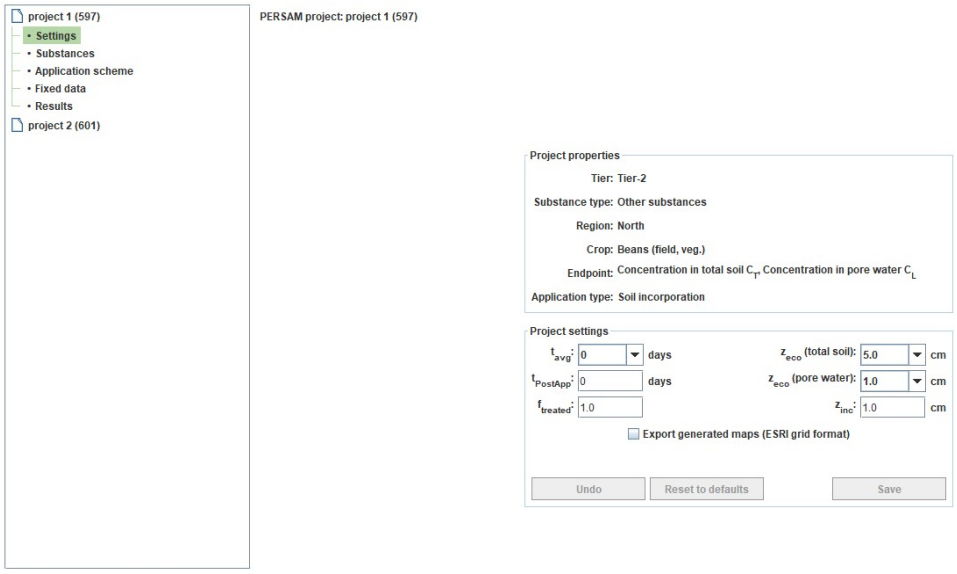
In case you want to change the project properties, follow the next instructions:

1. Export the project to a JSON file
2. Change the project properties in the JSON file (see PERSAM 3 export/import file format)
3. Import the adapted JSON file
4. PERSAM creates a new project based on the file import.

Here you can find a few examples how to change the project properties.

5.3.1. Change zone and application type

In next project the zone and the application type should be updated.



First export this project to a JSON file and open this export file.


```
{
 "name" : "project 1",
 "outputFolder" : "C:\\Users\\decortel\\OneDrive - VITO\\Documents\\persam\\exports",
 "properties" : {
  "tier" : "tier2",
  "substanceType" : "other",
  "regionType" : "zone",
  "regions" : [ "north" ],
  "cropType" : "annual",
  "crop" : "beans",
  "endpoints" : [ "totalSoil", "poreWater" ],
  "applicationType" : "soilIncorporation"
 },
 "settings" : {
  "exportGeneratedMaps" : false,
  "zecoTotalSoil" : 5.0,
  "zecoPoreWater" : 1.0,
  "ftreated" : 1.0,
  "tpostApp" : 0,
  "zinc" : 1.0,
  "tavg" : 0
 },
 "substanceTree" : {
  "parentSubstance" : {
   "substanceDefinition" : "predefined1",
   "code" : "substance 1",
   "kom" : 10.0,
   "degT50" : 10.0,
   "m" : 300.0,
   "e" : 65.4,
   "racTotalSoil" : 10.0,
   "racPoreWater" : 15.0
  }, ...
```

Change the yellow lines into the new values. See section 13.11.5 for the project properties.


```
{
 "name" : "project 1",
 "outputFolder" : "C:\\Users\\ persam\\exports",
 "properties" : {
  "tier" : "tier2",
  "substanceType" : "other",
  "regionType" : "zone",
  "regions" : [ "north", "South" ],
  "cropType" : "annual",
  "crop" : "beans",
  "endpoints" : [ "totalSoil", "poreWater" ],
  "applicationType" : "soilDepth"
 },
 "settings" : {
  "exportGeneratedMaps" : false,
  "zecoTotalSoil" : 5.0,
  "zecoPoreWater" : 1.0,
  "ftreated" : 1.0,
  "tpostApp" : 0,
  "zinc" : 1.0,
  "tavg" : 0
 },
 "substanceTree" : {
  "parentSubstance" : {
   "substanceDefinition" : "predefined1",
   "code" : "substance 1",
   "kom" : 10.0,
   "degT50" : 10.0,
   "m" : 300.0,
   "e" : 65.4,
   "racTotalSoil" : 10.0,
   "racPoreWater" : 15.0
  }, …
```


Import the changed export file into PERSAM. PERSAM creates a new project based on the JSON file.

5.3.2. Change crop and endpoint

Export the project to a JSON file and open this file. Change the settings of substance type and crop in the project object (see section 13.11.5)

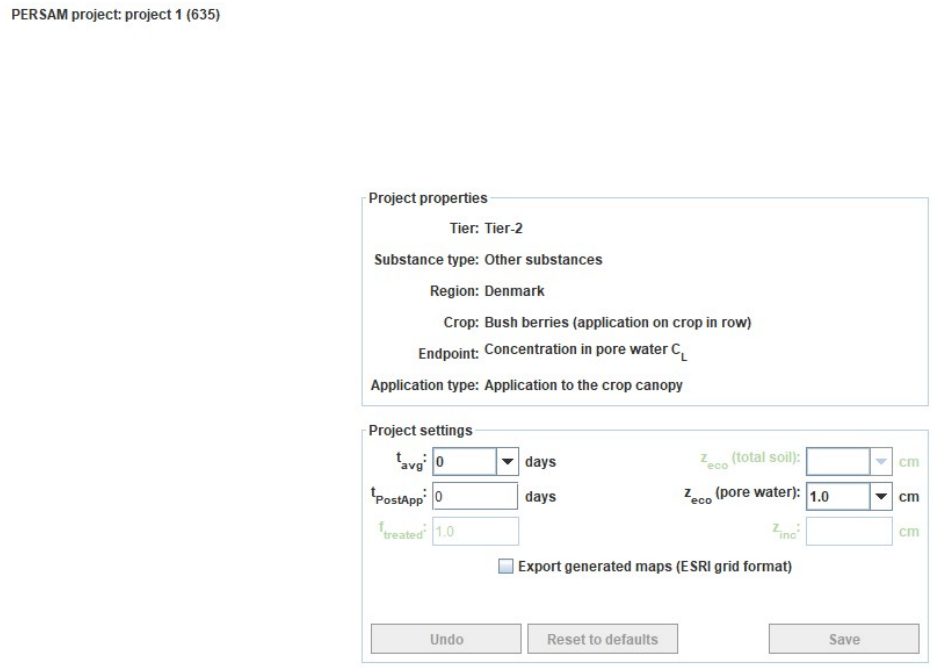

```
{
 "name" : "project 1",
 "outputFolder" : "C:\\Users\\persam\\exports",
 "properties" : {
  "tier" : "tier2",
  "substanceType" : "other",
  "regionType" : "euMemberState",
  "regions" : [ "Denmark" ],
  "cropType" : "permanent",
  "crop" : "applesInRow",
  "endpoints" : [ "totalSoil", "poreWater" ],
```

```
  "applicationType" : "cropCanopy"
 }
```

Changed JSON file:

```
{
 "name" : "project 1",
 "outputFolder" : "C:\\Users\\persam\\exports",
 "properties" : {
  "tier" : "tier2",
  "substanceType" : "other",
  "regionType" : "euMemberState",
  "regions" : [ "Denmark" ],
  "cropType" : "permanent",
  "crop" : "bushBerriesInRow",
  "endpoints" : ["poreWater" ],
  "applicationType" : "cropCanopy"
 }
```

Import this JSON file into PERSAM and PERSAM creates a new project based on this file.



6. Substances

Substances are organized in a tree structure. The root of this tree contains the parent substance. The tool allows the definition of up to 2 levels of metabolites: substances that are formed out of substances in the level above them. Each level can contain up to 4 metabolites.

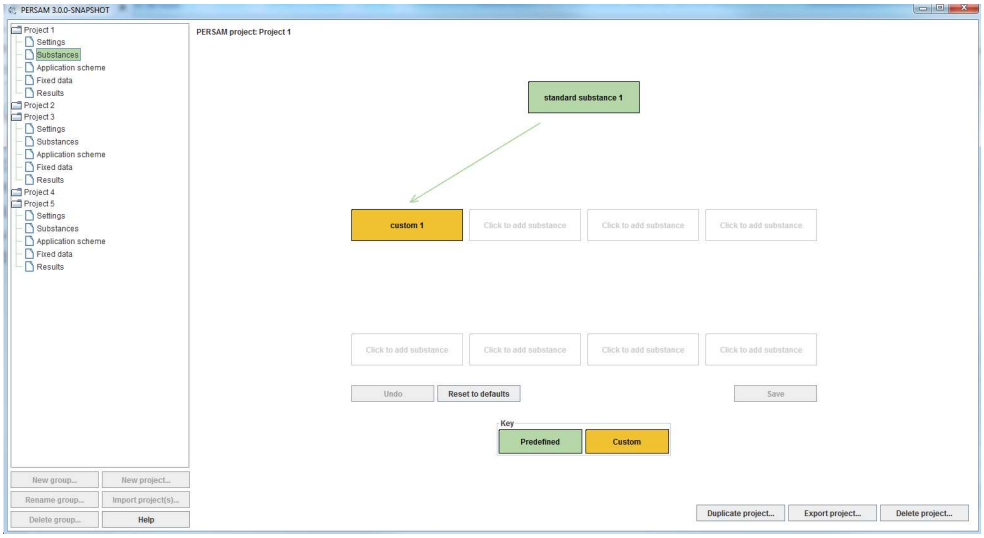


Figure 31: Substances section

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 colour of the place holders indicates which of those 2 types of substances is used. Arrows between the place holders can be configured by clicking on them.

Only the arrows between place holders that contain a substance can be configured.

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

Table 3: Substance-specific parameters

	Symbol	Unit	Default value
Parameter			
Half-life for degradation of the	DegT50	days	
Organic matter/water	K_{om}	l/kg	
Organic carbon/water	K_{oc}	ml/g	
Molar mass	M	$g.mol^{-1}$	
Arrhenius activation energy	E	$kJ.mol^{-1}$	65.4

Related functionalities:

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

6.1. Configure predefined substance

The user defines a predefined substance (parent or metabolite)

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

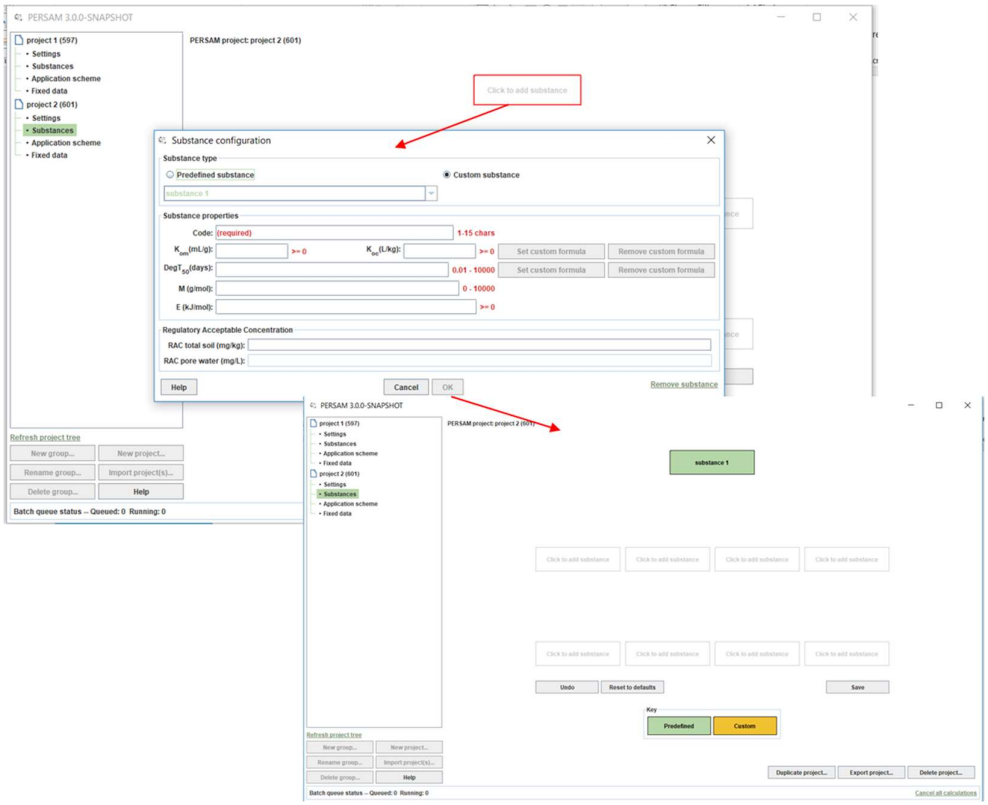


Figure 32: Configure a predefined substance (parent or metabolite)

6.2. Configure custom substance

The user defines a customized substance (parent or metabolite) .

1. Click on a place holder in the tree and the screen 'Configure substance' appears.
2. Select 'Custom substance'
3. Define the code and the substance related parameters.
4. Click on 'OK'

For microbial substances, M and E are disabled

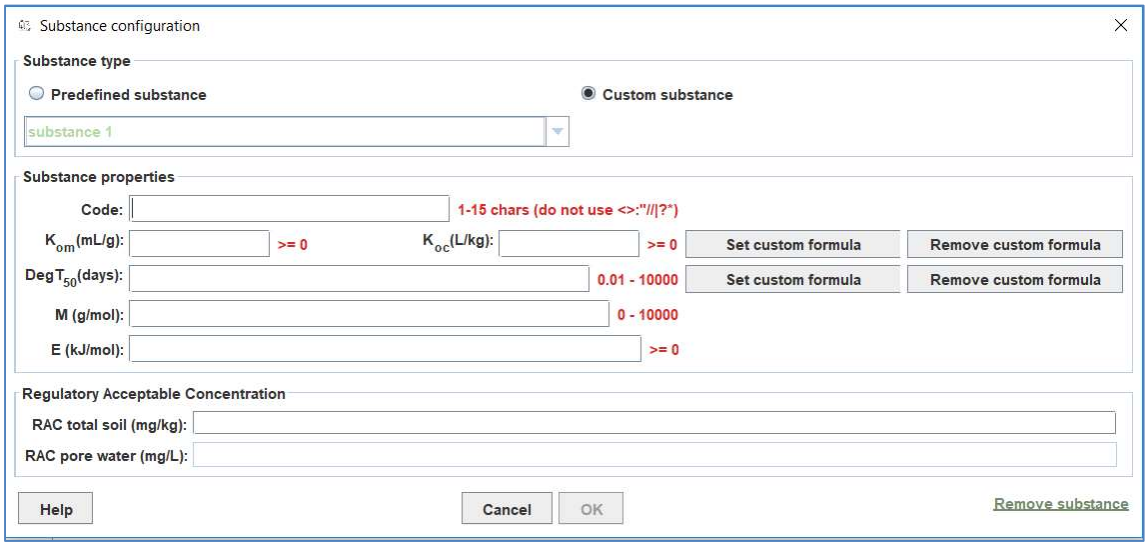


Figure 33: Substance configuration

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

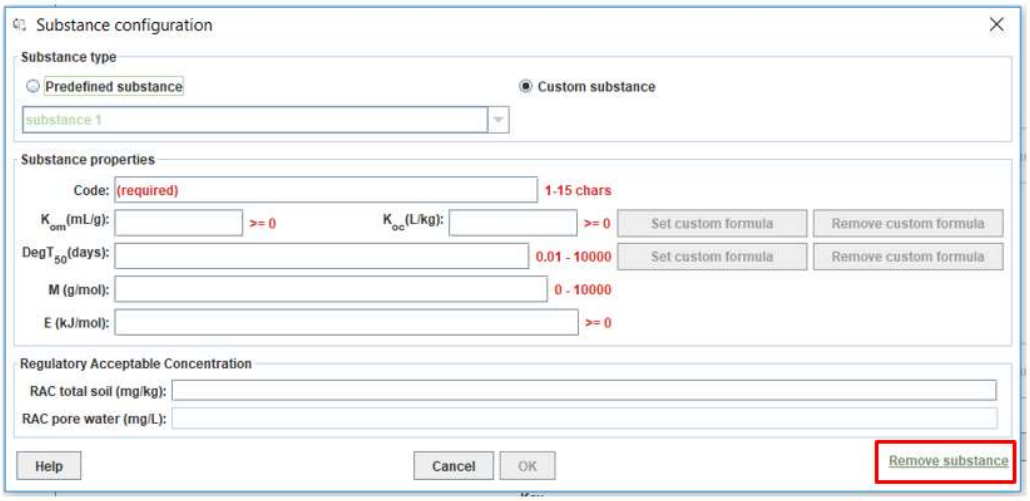


Figure 34: Delete a configured substance

6.4. Configure link

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

1. Click on an arrow between two place holders that contain a substance and the dialog 'Link configuration' appears. The precursor and the metabolite are informative: they cannot be changed.
2. Define the formation factor
3. Click 'OK'

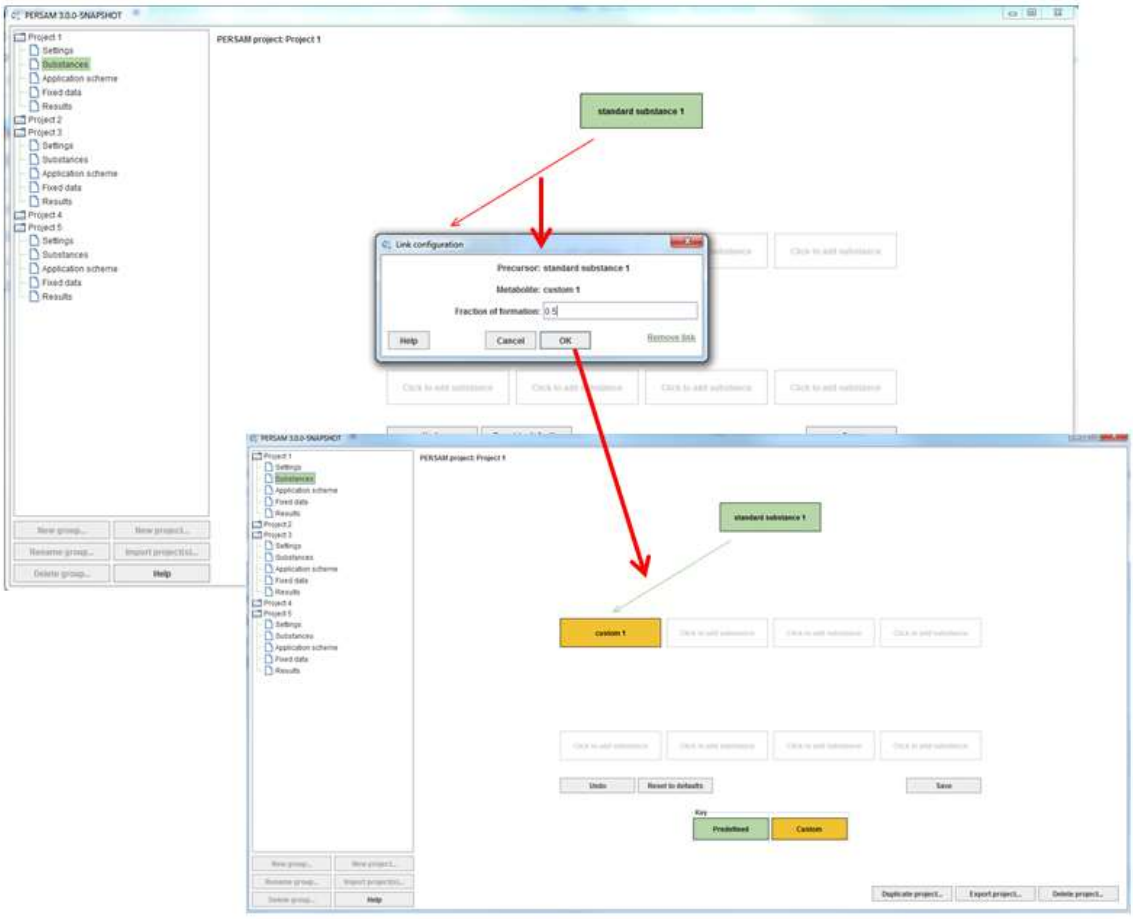


Figure 35: Configure a link

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

6.5. 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. Click on 'Remove link'
3. Click on 'OK' and the arrow is removed in the substance tree.

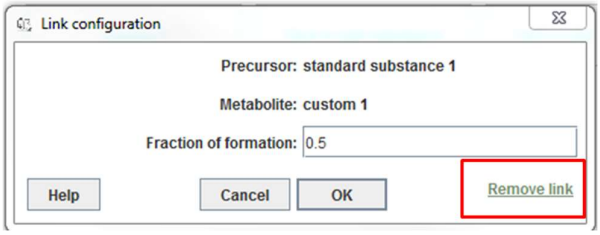


Figure 36: Delete a link

6.6. Configure custom calculations

The user has the possibility to define relationships between Kom, DegT50 and soil properties. This functionality is only available for Ter-2 and Tier-3A.

Configure a custom calculation for Kom or for DegT50

1. Click on a place holder in the tree and the screen 'Substance configuration' appears.
2. Configure a predefined substance (see Configure predefined substance) or a custom substance (see Configure custom substance)
3. Click on 'Set custom formule' of K_{om} or $DegT_{50}$ and the dialog 'Define custom calculation' appears
4. Select the calculation type by clicking on 'Custom formula' or 'pH dependent sorption'

(a) Calculation based on custom formula:

1. Select a spatial parameter by clicking on 'fraction of organic matter' or 'pH' or enter the related label 'clay' or 'pH'
2. Select an operator

Table 4: Spatial parameters available in 'Custom formula

	Code
Spatial parameter	
Fraction of clay (kg/kg)	[clay]
pH (pH)	[ph]

3. Select another parameter or enter a value in the formula rectangle.
4. Limit K_{om}/$DegT_{50}$ to user min and max values, if necessary

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

5. Click on 'OK'

(b) Calculation based on pH dependent sorption:

1. Enter the parameters related to pH dependent sorption

   Formula for pH dependent sorption:

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

   pKa: negative logarithm of the dissociation constant

   pH: pH correction factor

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

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

2. Click 'OK'.

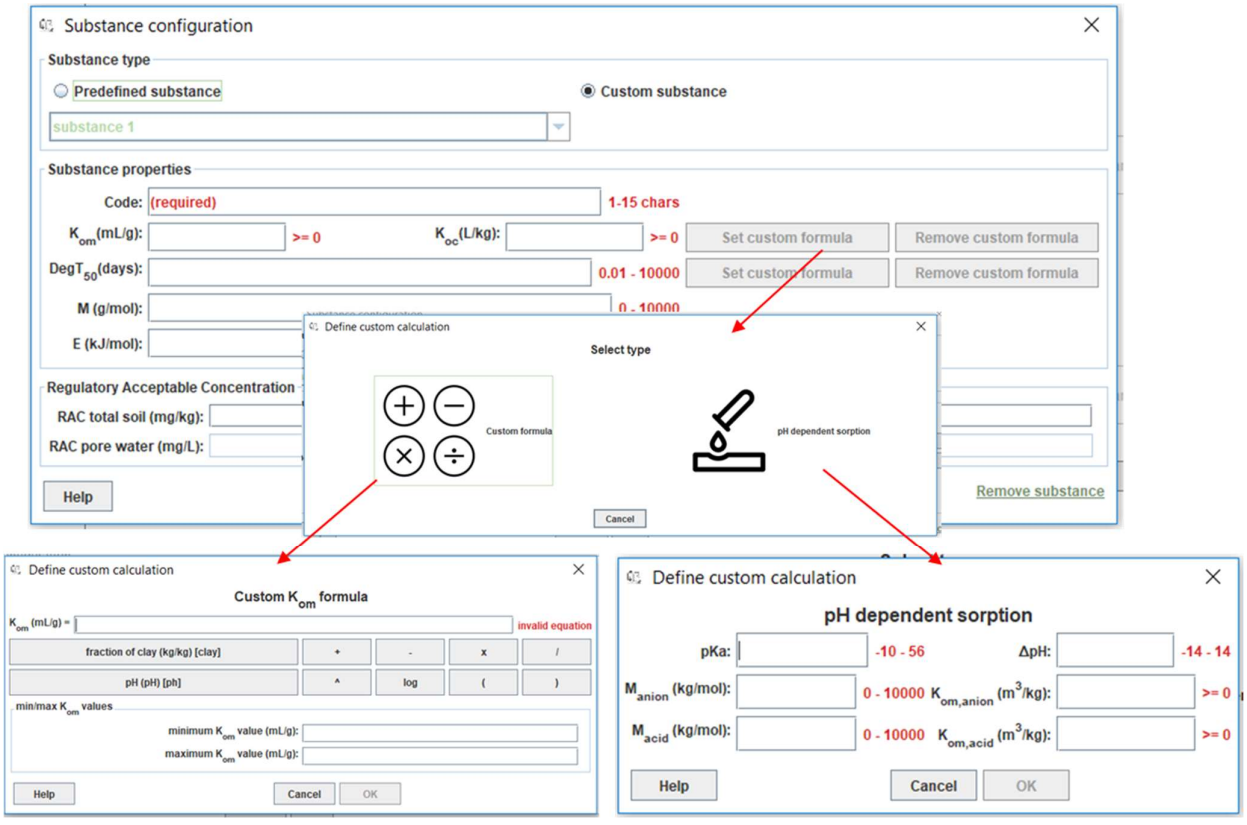


Figure 37: Define custom calculation for K_{om}

7. Application scheme

The application scheme is dependent on the selected substance type. If 'other substances' is selected as substance type the user defines the application(s), the time since first application and the crop development stage/season.

1. Define the application parameters: application rate in kg/ha, Time since first application (dt) and the crop development stage/season (BBCH code or time interval). In case citrus, olives, permanent grass or grass between rows is selected as focus crop, the crop development stage contains the intervals Jan-Mar, Apr-Jun, Jul-Sep, Oct-Dec instead of the BBCH code. The crop development stage is only required for Tier-2 and Tier-3A.
2. Click on 'Add to table'. The application is added to the table. You can **delete an application** by clicking on the cross action of a particular application
3. Define the period of crop rotation in years. The default value in 1 year.

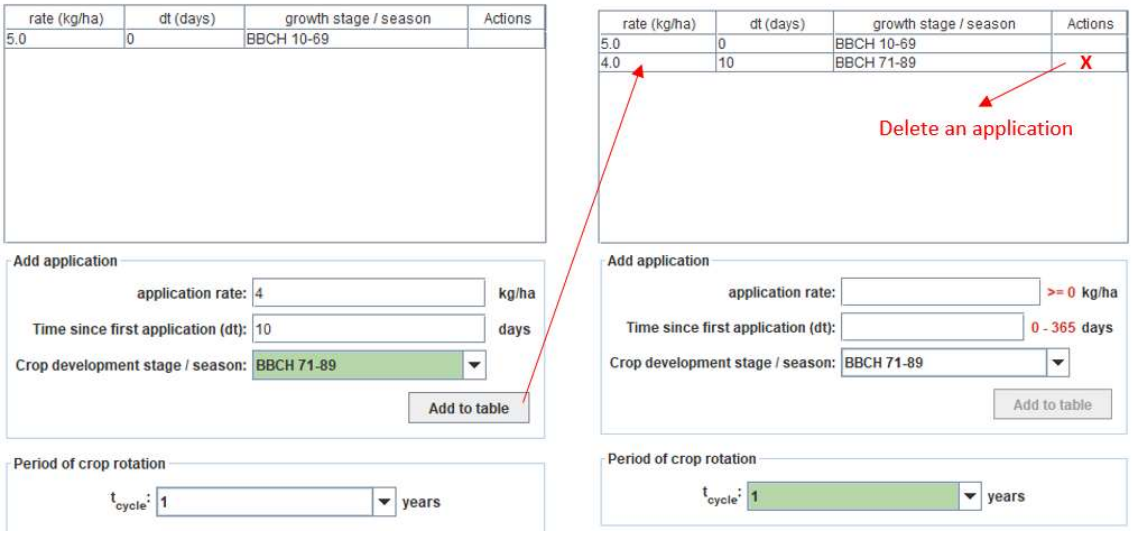


Figure 38: Application scheme

The user can also **update** the information of one particular application in the application scheme.

1. Place the cursor on the application to be updated
2. Enter the application rate and the time since first application, and if necessary the crop development stage/season. Application rate and time since first application are required parameters.
3. Click on 'Add to table' and the selected application is updated.

The time since first application for the first application is always zero. When this application need to be updated enter zero as time since last application otherwise a new application row is added to the first application can only be deleted when there are no other applications defined in the application table. The user can **delete** the first application in the application scheme.

1. Remove first other applications so that there is only one application in the application scheme
2. Delete the first application by clicking on the cross in the application scheme.

If '**microbial active substance**' is selected the application dose in CFU/ha and number of applications are required parameters.

Figure 39: Required parameters for microbial active substance in the application scheme

8. Fixed data

This screen gives an overview of the fixed data used by PERSAM in the calculations. All parameters are not editable in the screen. The fixed data used in the calculations is dependent on the selected tier.

8.1. Tier-1: Fixed data

This screen gives an overview of the fixed data used by PERSAM in the calculations. All parameters are not editable in the screen. The fixed data used in the calculations is dependent on the selected tier. Table below describes the parameters of the fixed data for Tier-1. When microbial substance is selected, the adjustment scenario and model factors are **not used** in the calculations.

Table 5: Parameters of Tier-1 fixed data screen

Symbol	Unit	Description
T_{arit}	°C	°C Temperature T_{arit}
T_{arr}	°C	°C Temperature T_{arr}
θ_{fc}	$m^3\ m^{-3}\theta_{fc}$	volume fraction of liquid in soil at field capacity
ρ	$Kg\ L^{-1}$	Dry bulk density
f_{om} Organic matter content	$kg.kg^{-1}$	Organic matter content
fs		Adjustment scenario factor
fM	°C	Adjustment model factor
Tref		Reference temperature
R	$kJ.mol^{-1}.K^{-1}$	Gas contstant

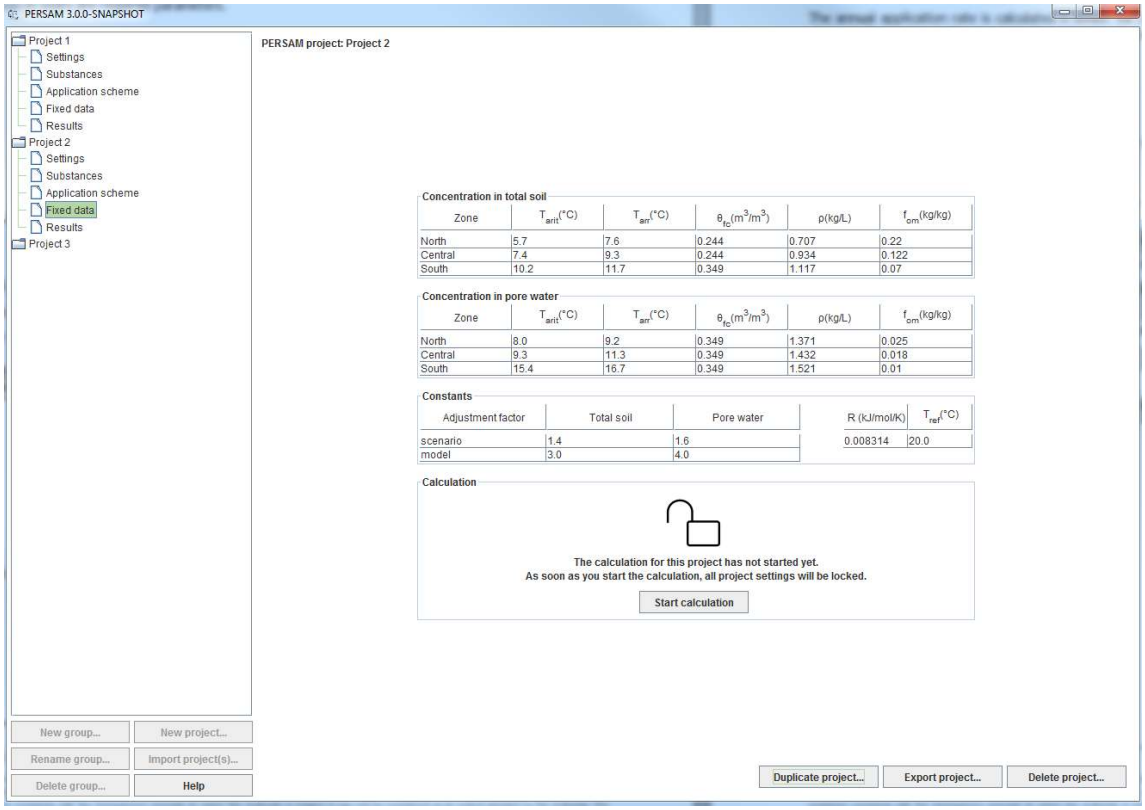


Figure 40: Tier-1: Fixed data

The Tier-1 calculations can be started by clicking on the 'Start calculation' button in the Fixed data screen.

8.1. Tier-2 & Tier-3A: Fixed data

This screen gives an overview of the fixed data used by PERSAM 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 (f_{om} in kg/kg)
- Fraction of clay (f_{clay} in kg/kg)
- pH

Table below describes the fixed parameters for Tier-2, used in the calculations.

Table 6: Fixed parameters of Tier-2

Symbol	Unit	Description
fs		Adjustment scenario factor
fM		Adjustment model factor
Tref	°C	Reference temperature
R	$kJ.mol^{-1}.K^{-1}$	Gas contstant

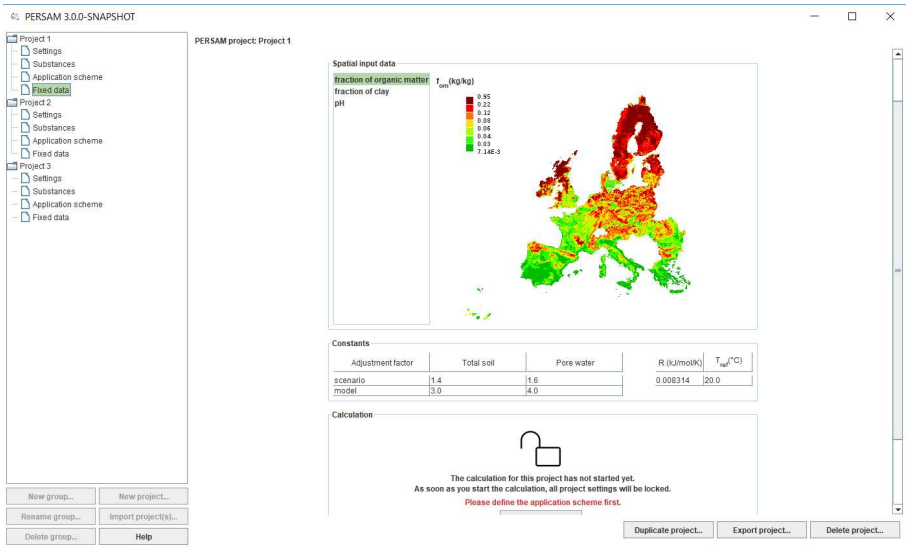


Figure 41: Tier-2: Fixed data

9. Calculations

This section describes the PERSAM calculations for the three tiers. The calculations can be started by clicking on the 'start calculation' button in the fixed data screen. As long as the calculations of a project are in progress, the clock is visible in the fixed data screen. When the calculation for a project are finished, the fixed data screen contains the message 'The calculation for this project is done' and the results screen is visible in the project.

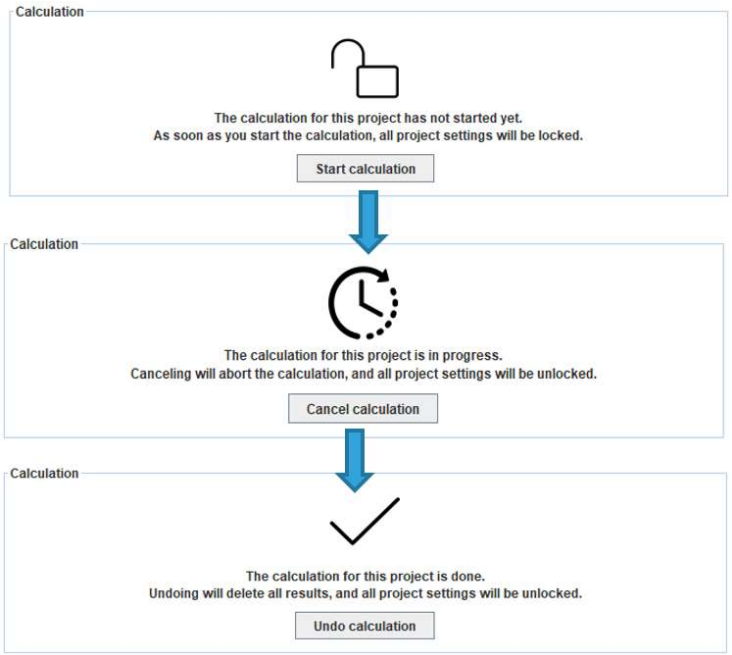


Figure 42: Performing calculations: status flow

9.1. Tier-1: Calculations

STEP 1: Calculate annual application rate for each substance

The annual application rate is calculated n times: for i = 1..1, i = 1..2, …, i = 1..n. The maximum of all these A_{year} values is then used as the value for the annual application rate.

Parent substance

Formula 1:

$$A_{year} = \sum_{i=1}^{n} \left(f_{soil,i} \cdot A_i \cdot e^{-f_T \cdot k_{ref} \cdot (t_{app,n} - t_{app,i})} \right)$$

Symbol	Unit	Description	Origin
A_{year}	kg/ha ≈ mg/dm^2	annual application rate	
n		number of applications	user provided
$f_{soil,i}$		fraction of the dose reaching the soil for application i	calculated
A_i	kg/ha	application rate of application i	user provided
f_T		see formula 7	calculated
k_{ref}		see formula 8	calculated
$t_{app,i}$	day index	day-of-year of application i	user provided

For Tier-1 (no crop interception):

Formula 2:

$$f_{soil} = 1.0$$

Metabolites

Formula 3:

$$A_{year} = \sum_{i=1}^{n} \left(f_{soil,i} \cdot A_i \cdot e^{-f_T \cdot k_{ref} \cdot (t_{app,n} - t_{app,i})} \cdot \frac{M_{met}}{M_{parent}} \sum_{j=1}^{m} \left(F_{f,p,j} \cdot F_{f,s,j} \right) \right)$$

Symbol	Unit	Description	Origin
A_{year}	kg/ha ≈ mg/dm^2	annual application rate	
n		number of applications	user provided
$f_{soil,i}$		fraction of the dose reaching the soil for application i	calculated
A_i	kg/ha	application rate of application i	user provided
f_T		see formula 7	calculated
k_{ref}		see formula 8	calculated

Symbol	Unit	Description	Origin
$t_{app,i}$	day index	day-of-year of application i	user provided
m		number of metabolite formation pathways	user provided
M_{met}	g/mol	Molar mass of the metabolite considered (primary or secondary)	user provided
M_{parent}	g/mol	Molar mass of the parent substance	user provided
$F_{f,p,j}$		formation fraction of the primary metabolite	user provided
$F_{f,s,j}$		formation fraction of the secondary metabolite	user provided

STEP 2: Rum simple analytical model for each substance, each t_{avg} and each endpoint

Initial concentration in total soil directly after the application:

Formula 4:

$$C_{T,ini} = \frac{A_{year}}{\rho \cdot z_{eco}}$$

Symbol	Unit	Description	Origin
A_{year}	kg/ha ≈ mg/dm^2	annual application rate	calculated
ρ	kg/dm^3	dry soil bulk density	Soil specific parameters – table 1 & 2 lookup table/spatial data
z_{eco}	dm	ecotoxicological averaging depth	user selected value out of list of fixed values (1,2.5,5,20)

Formula 5:

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

Symbol	unit	Description	Origin
z_{til}	dm	plough depth	fq, fom,corr, ztil, CT,ini and CT,plateau in relation to crop and application type – tables 1 & 2
X		See Formula 6	calculated
$f_{treated}$		fraction of the soil surface that is treated	Fixed at 1.0 in Tier-1

Formula 6:

$$X = e^{-t_{cycle} \cdot (f_T \cdot k_{ref} + k_{leach})}$$

Symbol	Unit	Description	Origin
t_{cycle}	days	time between applications (365, 730, or 1095 days)	user provided
f_T		see formula 7	calculated
k_{ref}	1/d	see formula 8	calculated
k_{leach}	1/d	see formula 9	calculated

Formula 7:

$$\begin{array}{ll} T > 0\,°C & f_T = e^{\frac{-E}{R}\left[\frac{1}{T+273.15}-\frac{1}{T_{ref}+273.15}\right]} \\ T \leq 0°C & f_T = 0 \end{array}$$

Symbol	Unit	Description	Origin
E	kJ/mol	Arrhenius activation energy	user provided
R	kJ/mol K	gas constant (0.008314)	fixed value
T	°C	soil temperature	lookup table/spatial data
T_{ref}	°C	temperature at reference conditions (20 °C)	fixed value

Formula 8:

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

Symbol	Unit	Description	Origin
$DegT_{50}$	days	degradation half-life in soil at reference temperature	user provided

Formula 9:

$$k_{leac} = \frac{q}{z_{eco} \cdot (\theta + \rho \cdot f_{om} \cdot K_{om})}$$

Symbol	Unit	Description	Origin
q	dm/d	mean annual downward water flow rate at the bottom of the layer	calculated
z_{eco}	dm	ecotoxicological averaging depth	user selected value out of list of fixed values
θ	m^3/m^3	volume fraction of liquid in soil at field capacity	Soil specific parameters table 1 & 2 lookup table/spatial data
ρ	kg/dm^3	dry soil bulk density	Soil specific parameters table 1 & 2 lookup table/spatial data

Symbol	Unit	Description	Origin
f_{om}	kg/kg	mass fraction of organic matter	Soil specific parameters table 1 & 2 lookup table/spatial data + correction (*)
K_{om}	ml/g	coefficient for sorption on organic matter	user provided

(*) For *annual crops*: $f_{om,corr}$ = 1; For *permanent crops*: use Appendix E table E.3 column 'Correction factor for situations without mechanical cultivation'

Formula 10:

$$q = f_q \cdot (P + I)$$

Symbol	Unit	Description	Origin
f_q		ratio of q and precipitation + irrigation	Soil specific parameters table 4
P + I	mm	mean annual precipitation + irrigation	Crop specification list table 1 /spatial data

Maximum concentration in total soil:

Formula 11:

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

Maximum concentration in the liquid phase:

Formula 12:

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

TWA concentrations:

Formula 13:

$$C_{?,TWA} = \frac{C_{?,peak}}{t_{avg} \cdot f_T \cdot k_{ref}} \cdot \left[1 - e^{-t_{avg} \cdot f_T \cdot k_{ref}}\right]$$

? = T (total soil) or L (liquid phase)

Symbol	Unit	Description	Origin
t_{avg}	days	time period since application time over which concentrations are averaged	user selected value out of list of fixed values (0; 1; 2; 3; 4; 7; 14; 21; 56; 100)

STEP 3: Apply scenario adjustment factor

Scenario and model adjustment factors table 5

STEP 4: Apply model adjustment factor

Scenario and model adjustment factors table C.6

STEP 5: Generate report

IMPACT OF MICROBIAL ACTIVE SUBSTANCE

a. Do NOT apply model adjustment factor
b. Only concentration in total soil endpoint is available
c. Annual total dose in CFU/ha must be specified as a single application, which will be converted to kg/ha by applying a factor 1.0/1e-6
d. K_{oc} is fixed at 2000 mL/g (== K_{om} fixed at 2000 / 1.724 L/kg)
e. M is 300g/mol and is fixed
f. f_T is 1
g. $DegT_{50}$ = 1000 days by default, but can be changed by the user

   DT50 is a geometric mean.
h. Calculated PECs must be converted from mg/kg to CFU/kg by applying a factor 1e-6 (no additional factor 1/3 "to cancel out model adjustment factor" because it isn't applied in this case)
i. PERSAM assumes no crop interception as the default (Tier-1) for Microbial active substances.

9.2. Tier-2: Calculations

STEP 1: Calculate annual application rate for each substance

The annual application rate is calculated n times: for i = 1..1, i = 1..2, …, i = 1..n. The maximum of all these A_{year} values is then used as the value for the annual application rate.

Parent substance

Formula 1:

$$A_{year} = \sum_{i=1}^{n} \left(f_{soil,i} \cdot A_i \cdot e^{-f_T \cdot k_{ref} \left(t_{app,n} - t_{app,i} \right)} \right)$$

Symbol	Unit	Description	Origin
A_{year}	kg/ha ≈ mg/dm^2	annual application rate	
n		number of applications	user provided
$f_{soil,i}$		fraction of the dose reaching the soil for application i	calculated
A_i	kg/ha	application rate of application i	user provided
f_T		see formula 9	calculated

Symbol	Unit	Description	Origin
k_{ref}		see formula 10	calculated
$t_{app,i}$	day index	day-of-year of application i	user provided

For Tier-2 and Tier-3A:

Formula 2:

$$f_{soil} = (1 - f_i) + f_i \cdot f_w$$

Symbol	Unit	Description	Origin
f_i		fraction of the dose intercepted	Crop interception factors – tables 1 & 2 (*)
f_w		wash-off fraction of the dose intercepted by the crop canopy	Appendix B – tables B.1 & B.2 (*)
BBCH		code (0-99) characterising the crop development stage	user provided

(*) When fi and/or fw value are not present in tables, use the crop in PERSAM with the highest scenario adjustment factor.(see Scenario and model adjustment factors – tables 1 → 4)

Metabolites

Formula 3:

$$A_{year} = \sum_{i=1}^{n} \left(f_{soil,i} \cdot A_i \cdot e^{-f_T \cdot k_{ref} \cdot (t_{app,n} - t_{app,i})} \cdot \frac{M_{met}}{M_{parent}} \sum_{j=1}^{m} (F_{f,p,j} \cdot F_{f,s,j}) \right)$$

Symbol	Unit	Description	Origin
A_{year}	kg/ha ≈ mg/dm^2	annual application rate	
n		number of applications	user provided
$f_{soil,i}$		fraction of the dose reaching the soil for application i	calculated
A_i	kg/ha	application rate of application i	user provided
f_T		see formula 9	calculated
k_{ref}		see formula 10	calculated
$t_{app,i}$	day index	day-of-year of application i	user provided
m		number of metabolite formation pathways	user provided
M_{met}	g/mol	Molar mass of the metabolite considered (primary or secondary)	user provided
M_{parent}	g/mol	Molar mass of the parent substance	user provided
$F_{f,p,j}$		formation fraction of the primary metabolite	user provided
$F_{f,s,j}$		formation fraction of the secondary metabolite	user provided

STEP 2: Run simple analytical model for each substance, each t_{avg}, each endpoint, in each cell where crop cover is above 1%, $T_{arr} > 0$, and all required soil parameters are available

Initial concentration in total soil directly after the application:

If application type = 'Soil incorporation' and $z_{inc} \geq z_{eco}$: use formula 4.

Formula 4:

$$C_{T,ini} = \frac{A_{year}}{\rho \cdot z_{inc}}$$

For all other case use formula 5.

Formula 5:

$$C_{T,ini} = \frac{A_{year}}{\rho \cdot z_{eco}}$$

Symbol	Unit	Description	Origin
A_{year}	kg/ha ≈ mg/dm^2	annual application rate	calculated
ρ	kg/dm^3	dry soil bulk density	Soil specific parameters – table 1 & 2 lookup table/spatial data
z_{eco}	dm	ecotoxicological averaging depth	user selected value out of list of fixed values (1,2.5,5,20)
z_{inc}	dm	incorporation depth (optional)	user provided

Background concentration just before the next application after an infinite number of annual applications:

For annual crops with application type = 'Soil incorporation' and $z_{inc} \geq z_{til}$: use formula 6

For permanent crops with application type = 'Soil incorporation' and no mechanical cultivation and $z_{inc} \geq z_{eco}$: use formula 6

For permanent crops with application type = 'Soil incorporation' and mechanical cultivation and $z_{inc} \geq z_{eco}$ and $z_{inc} \geq$ 5cm : use formula 6

Formula 6:

$$C_{T,plateau} = f_{treated} \cdot \frac{A_{year}}{\rho \cdot z_{inc}} \cdot \frac{X}{1 - X}$$

For all other cases use formula 7.

Formula 7:

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

Symbol	Unit	Description	Origin
z_{til}	dm	plough depth	f_q, $f_{om,corr}$, z_{til}, $C_{T,ini}$ and $C_{T,plateau}$ in relation to crop and application type – tables 1 & 2
X		See Formula 8	calculated
$f_{treated}$		fraction of the soil surface that is treated	Default 1.0 (*)

(*) For permanent crops is $f_{treated}$ fixed and 1.0; For annuals crops f treated is user input except for potatoes.

Formula 8:

$$X = e^{-t_{cycle} \cdot (f_T \cdot k_{ref} + k_{leach})}$$

Symbol	Unit	Description	Origin
t_{cycle}	days	time between applications (365, 730, or 1095 days)	user provided
f_T		see formula 9	calculated
k_{ref}	1/d	see formula 10	calculated
k_{leach}	1/d	see formula 11	calculated

Formula 9:

$$\begin{array}{ll} T > 0\,°C & f_T = e^{\frac{-E}{R}\left[\frac{1}{T+273.15} - \frac{1}{T_{ref}+273.15}\right]} \\ T \leq 0°C & f_T = 0 \end{array}$$

Symbol	Unit	Description	Origin
E	kJ/mol	Arrhenius activation energy	user provided
R	kJ/mol K	gas constant (0.008314)	fixed value
T	°C	soil temperature	lookup table/spatial data
T_{ref}	°C	temperature at reference conditions (20 °C)	fixed value

Formula 10:

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

Symbol	Unit	Description	Origin
$DegT_{50}$	days	degradation half-life in soil at reference temperature	user provided

Formula 11:

$$k_{leach} = \frac{q}{z_{eco} \cdot (\theta + \rho \cdot f_{om} \cdot K_{om})}$$

Symbol	Unit	Description	Origin
q	dm/d	mean annual downward water flow rate at the bottom of the layer	calculated
z_{eco}	dm	ecotoxicological averaging depth	user selected value out of list of fixed values
θ	m^3/m^3	volume fraction of liquid in soil at field capacity	Soil specific parameters table 1 & 2 lookup table/spatial data
ρ	kg/dm^3	dry soil bulk density	Soil specific parameters table 1 & 2 lookup table/spatial data
f_{om}	kg/kg	mass fraction of organic matter	Soil specific parameters table 1 & 2 lookup table/spatial data + correction (*)
K_{om}	ml/g	coefficient for sorption on organic matter	user provided

(*) f_{om} is corrected by multiplying with $f_{om,corr}$ = weighted average of the scaling factor values in table 3 of f_q, $f_{om,corr}$, z_{til}, $C_{T,ini}$ and $C_{T,plateau}$ in relation to crop and application type from soil depth A to B.
If application type = 'Placing at a certain soil depth' then A = z_{inc} and B = z_{inc} + z_{eco}.
In all other cases A = 0 and B = z_{eco}.

Formula 12:

$$q = f_q \cdot (P + I)$$

Symbol	Unit	Description	Origin
f_q		ratio of q and precipitation + irrigation	Soil specific parameters table 4 (*)
P + I	mm	mean annual precipitation + irrigation	Crop specification list table 1 /spatial data

(*) If application type = 'Placing at a certain soil depth', the reference depth to use in lookup table 4 of Soil specific parameters, is set at z_{eco} + z_{inc}. If this value lies between the predefined values 1, 2.5, 5, 20 cm, the lower value needs to be used as reference depth. For example: if z_{eco} + z_{inc} = 15 cm, use 5 cm. In all other cases, z_{eco} has to be used as reference depth in lookup table 4 of Soil specific parameters

Maximum concentration in total soil:

Formula 13:

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

Maximum concentration in the liquid phase:

Formula 14:

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

TWA concentrations:

Formula 15:

$$C_{?,TWA} = \frac{C_{?,peak}}{t_{avg} \cdot f_T \cdot k_{ref}} \cdot \left[1 - e^{-t_{avg} \cdot f_T \cdot k_{ref}}\right]$$

? = T (total soil) or L (liquid phase)

Symbol	Unit	Description	Origin
t_{avg}	days	time period since application time over which concentrations are averaged	user selected value out of list of fixed values (0; 1; 2; 3; 4; 7; 14; 21; 56; 100)

Post-application PEC values:

Formula 16:

$$C_{T,post} = C_{T,peak} \exp\left(-t_{post} \left(f_T k_{ref} + k_{leach}\right)\right)$$

$$C_{L,post} = C_{L,peak} \exp\left(-t_{post} \left(f_T k_{ref} + k_{leach}\right)\right)$$

Symbol	Unit	Description	Origin
$C_{T, post}$		Post-application PEC value for total soil	Calculated formula 16
$\mathbf{C_{L,post}}$		Post-application PEC value for liquid phase	Calculated formula 16
$\mathbf{t_{post}}$	days	User-defined period	
$\mathbf{f_T}$		see formula 9	calculated
$\mathbf{k_{ref}}$	1/d	see formula 10	calculated
$\mathbf{k_{leach}}$	1/d	see formula 11	calculated

Remark: t_{post} is equal to IntPostApp. The peak concentrations are based on z_{eco}=20cm

STEP 3: Apply model adjustment factor

Scenario and model adjustment factors table 6

STEP 4: Write PEC/peak/plateau values in ascii grid and png format for each substance, each t_{avg}, and each endpoint

STEP 5: If member state is provided: generate risk map (asci grid and png format) for each substance, each t_{avg}, and each endpoint: PEC > RAC red, PEC < RAC green

STEP 6: Calculate CFD values for each zone or the member state, for each substance, each t_{avg} and each endpoint

STEP 7: Calculate 95the percentile for each zone or in the member state, for each substance, each t_{avg} and each endpoint

STEP 8: Generate report for each substance, each t_{avg}, and each endpoint

STEP 9: Generate extended report for Tier-2

IMPACT OF MICROBIAL ACTIVE SUBSTANCE

The possibility to carry out a Tier-2 for microbial PPPs consists of accounting for crop interception to reduce the CFU calculated to be in the soil. When experimental data are available, the dose rate input into PERSAM in CFU/ha is reduced. However, this is something the user needs to do **outside of the tool, and use this as input in a PERSAM Tier-1 calculation**. A 'classical' Tier-2 for microbial PPPs is not available.

9.3. Tier-3A: Calculations

STEP 1: Calculate the refinement factor f_{ref}:

$$f_{ref} = \frac{\frac{z_{eco}}{z_{til}} \cdot \frac{X}{1-X} \cdot f_{treated} + 1}{\frac{z_{eco}}{z_{til}} \cdot \frac{X}{1-X} + 1}$$

STEP 2: For each Tier-2 $C_{T/L,peak}$ map (without model adjustment factor applied (Appendix C - table C.6)):

a. Select all cells within the 94th – 96th percentile of the map
b. Calculate for this subset of cells the median value for:
   i. Temperature
   ii. Precipitation + irrigation
   iii. f_{om}
   iv. pH (if applicable)
   v. clay content (if applicable)
c. Select the coordinates of the cell for which O is minimal

$$O = \sum_{i=1}^{n} \left| \frac{p_i - p_{50}}{p_{50}} \right|$$

With p_i is property i (one of temperature, P+I, F_{om}, or pH), p_{50} is the median of these properties, n is the number of properties

Remark:

In case only a limited number of cells contain the crop for which the assessment is carried out, it can be that not all percentile intervals contain cells. According to the calculation procedure, for the Tier-3A scenario selection the cells between the 94th and 96th (area weighted) percentile must be used. If for example the crop coverage is 4 cells, it can be that cell 1 is the 10th percentile, cell 2 the 34th percentile, cell 3 the 68th percentile and cell 4 the 100th percentile. In this case, the 94-96 percentile interval is completely between cell 3 and cell 4. PERSAM will then select the cell just above the interval to build the Tier-3A scenario, which is cell 4 in the example.

STEP 3: Generate transfer files

Generate transfer file for each substance, for each endpoint, and for each zone (in case of member state calculation: for the zone in which the member state is located)

STEP 4: Generate report for each substance, and each endpoint

STEP 5: Generate extended report for Tier-3A

10. Results

When the calculations are finished, the results can be viewed in the results screen. The results are dependent on the selected tier.

10.1. Tier-1: Results

When the calculations are finished, the results can be viewed in the results screen.

1. Select a particular zone and/ or a particular endpoint
2. The results are visible in the table below
   The table shows always the calculated results for the default settings and the user defined settings.

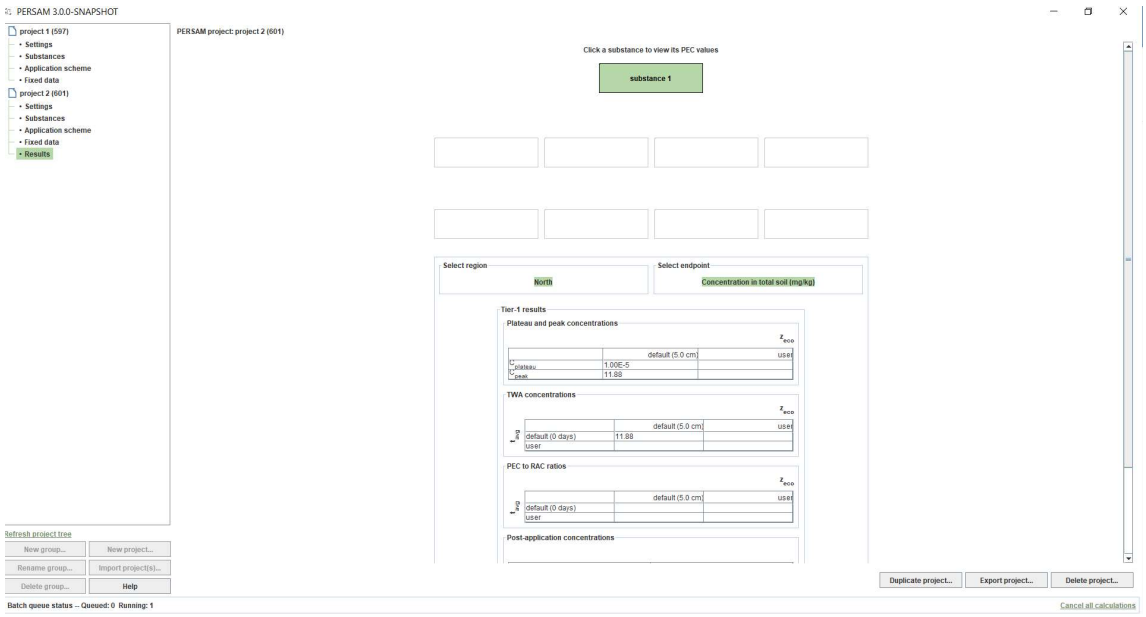


Figure 43: Tier-1: Results

10.2. Tier-2 & Tier-3A: Results

When the calculations are finished, the results of Tier-2 and Tier-3A are presented in the results screen.

Results of Tier-2:

1. Select a particular zone and/ or a particular endpoint
2. The results are visible in the table below
3. Click on a particular cell to see the spatial data

The table shows always the calculated results for the default settings and the user defined settings

Figure 44: Tier-2: Results for concentration in total soil

Selecting the endpoint 'concentration in pore water' gives following results:

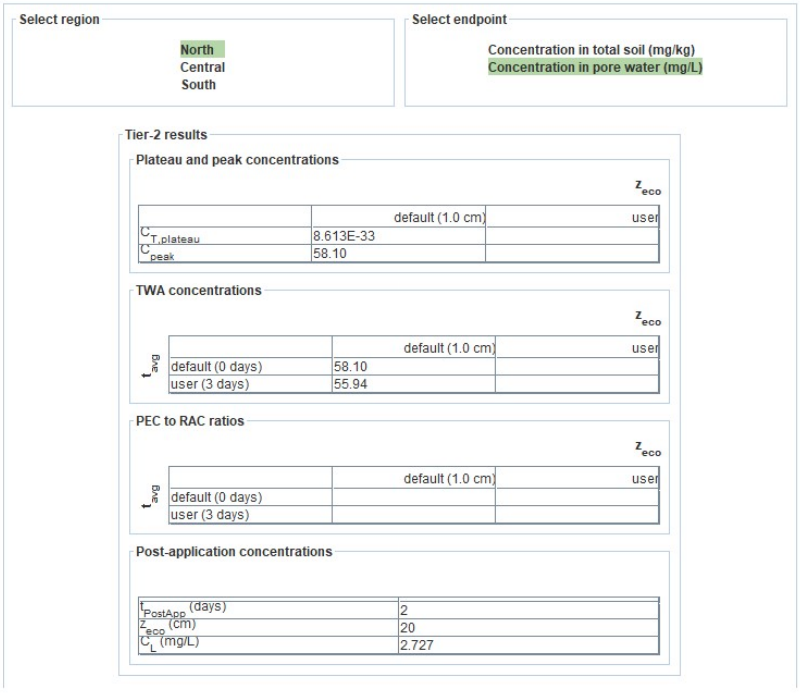


Figure 45: Tier-2: Results for concentration in pore water

In the results table, the calculated PECs for different time windows as well as the $C_{T,plateau}$ are provided both for concentration in total soil and concentration in pore water (depending on which of the two is selected by the user). Currently the $C_{T,plateau}$ for the location which gives the 95th percentile pore water peak concentrations is not intended to be used for regulatory use. More information on the exposure-assessment goal can be found in section 1.2 of the Guidance Document.

Results of Tier-3A:

1. Scroll down in the results window
2. Click on the 'Scenario locations' for the detailed results
3. Click on 'Open transfer file' for viewing the generated transfer file. The PERSAM transfer file is always generated in the output folder of the project.

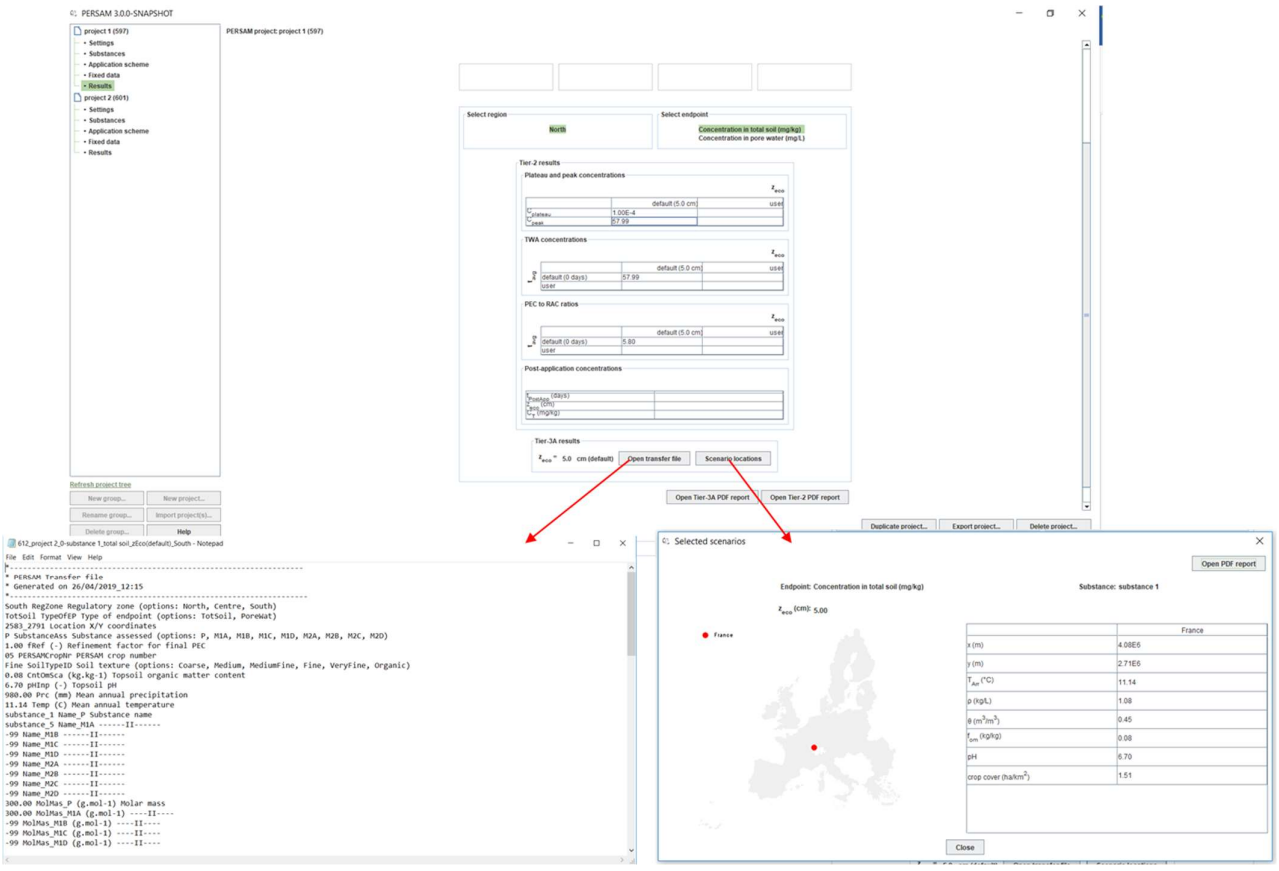


Figure 46: Tier-3: Results

11. Report management

PERSAM generates reports intended for regulatory submissions. Based on these reports the authorities need to be able to check or reproduce the model results.

There are two kind or reports available:

- Advanced reports for Tier-1, Tier-2 and Tier-3A
- Short reports for Tier-2 and Tier-3A

11.1. Advanced reports

Advanced reports are available for Tier-1, Tier-2 and Tier-3. The advanced reports contain all parameters used in the calculations, all results and graphical data.

1. Go to the Results screen
2. Click on the 'Open PDF report' button to view the pdf report
3. Click on 'Open output folder' to view reports in Word format

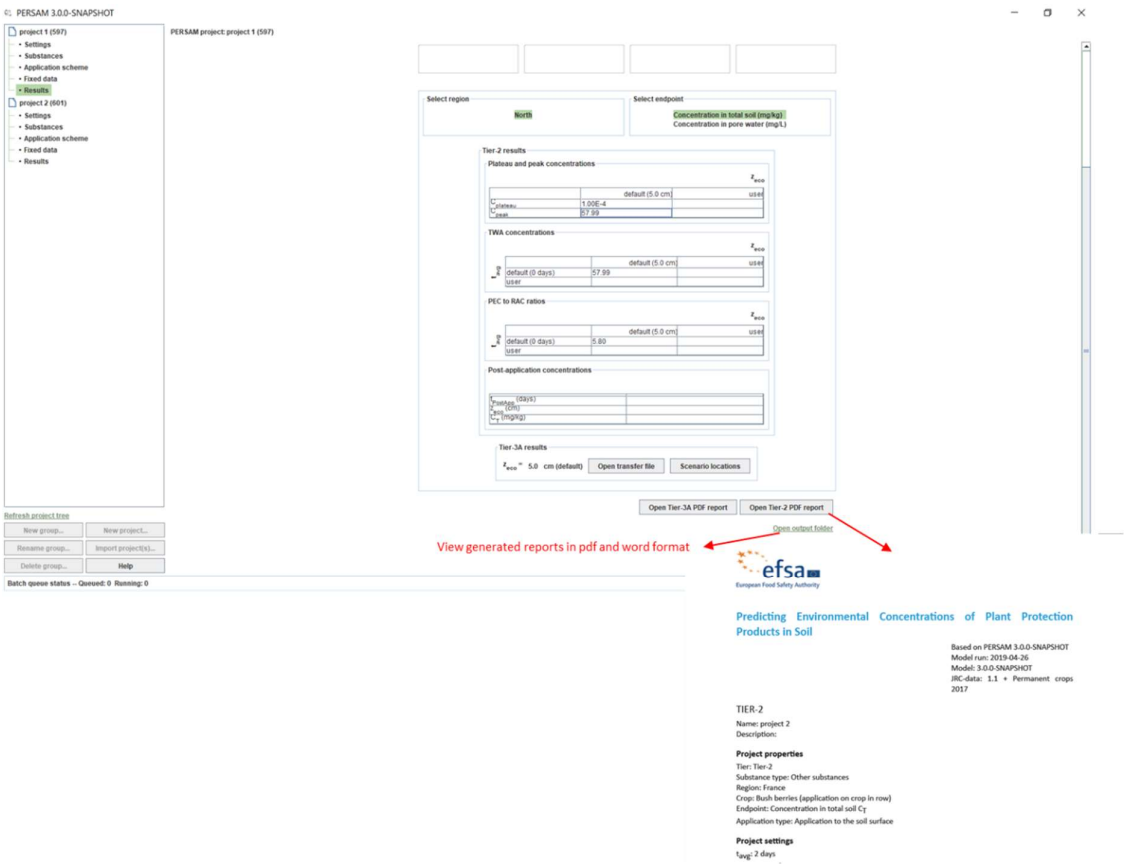


Figure 47: Advanced report

11.2. Short report

Short reports are available for Tier-2 and Tier-3A. The short report contains all parameters used in the calculations and the result and graphical data related to one cell in the results table.

1. Go to the Results screen
2. Click in a cell to view the detail results
3. Click on 'Open PDF report' to view the related short report

Reports in word format are available in the output folder of the project.

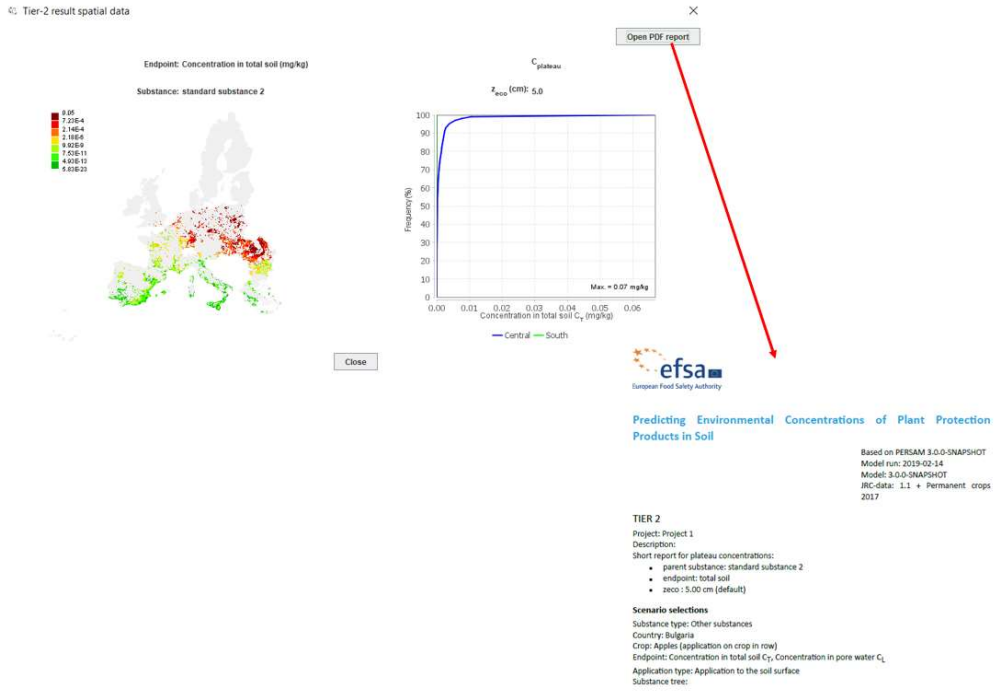


Figure 48: Short report

12. Batch processing

12.1. Batch mode

PERSAM provides the possibility to perform calculations in batch mode.

Import one or more projects. PERSAM only accepts JSON files. Check your JSON format file with the PERSAM 3 export/import file format (section 13.11). During the import process there is a possibility to start the calculations in batch mode. As long as the calculations of a project are in progress, the clock is visible in the fixed data screen. When the calculation for a project are finished, the fixed data screen contains the message 'The calculation for this project is done' and the results screen is visible in the project.

Figure 49: Performing calculations – status flow

12.2. Import multiple projects

PERSAM allows to import multiple projects in one time. The JSON file consists of several projects.

The main element in the export file is a list of (project) objects. A list in JSON is surrounded by []. An object in JSON is surrounded by {}. Items in a list in JSON are separated by a ,. An export file containing 2 empty projects looks as follows.

[{}, {}]

For the **first project**, use one export file (JSON) of project and change the settings (see section 13.11).

Next use another export file and change the settings. Copy and paste the **second project object** into the first export file according the described format.

```
[ {
  "name" : "project 2",
  "outputFolder" : "C:\\Users\\decortel\\OneDrive -
VITO\\Documents\\persam\\exports",
  "properties" : {
    "tier" : "tier1",
    "substanceType" : "other",
    "regions" : [ "north" ],
    "cropType" : "annual",
    "endpoints" : [ "totalSoil" ],
    "applicationType" : "soilSurface"
  },
  "settings" : {
    "exportGeneratedMaps" : false,
    "ftreated" : 1.0,
    "zecoTotalSoil" : 5.0,
    "zecoPoreWater" : 1.0,
    "tavg" : 0
  },
  "substanceTree" : {
    "parentSubstance" : {
      "substanceDefinition" : "predefined1",
      "code" : "substance 1",
      "kom" : 10.0,
      "degT50" : 10.0,
      "m" : 300.0,
      "e" : 65.4
    },
    "primaryMetabolites" : [ { }, { }, { }, { } ],
    "secondaryMetabolites" : [ { }, { }, { }, { } ],
    "primaryFormationFractions" : [ null, null, null, null ],
    "secondaryFormationFractions" : [ [ null, null, null, null ], [ null, null, null, null ], [
null, null, null, null ], [ null, null, null, null ] ]
  },
  "applicationScheme" : {
    "applications" : [ {
      "applicationRate" : 1.0,
      "dayIndex" : 0
    } ],
    "tcycle" : 1
  }
},
 {
  "name" : "test",
  "outputFolder" : "C:\\Users\\decortel\\OneDrive -
VITO\\Documents\\persam\\exports",
  "properties" : {
    "tier" : "tier2",
    "substanceType" : "other",
    "regionType" : "euMemberState",
    "regions" : [ "Denmark" ],
    "cropType" : "permanent",
    "crop" : "bushBerriesInRow",
    "endpoints" : [ "poreWater" ],
```

```
  "applicationType" : "cropCanopy"
 },
 "settings" : {
  "exportGeneratedMaps" : false,
  "tpostApp" : 0,
  "ftreated" : 1.0,
  "zecoTotalSoil" : 5.0,
  "zecoPoreWater" : 1.0,
  "tavg" : 0,
  "zinc" : 1.0
 },
 "substanceTree" : {
  "parentSubstance" : { },
  "primaryMetabolites" : [ { }, { }, { }, { } ],
  "secondaryMetabolites" : [ { }, { }, { }, { } ],
  "primaryFormationFractions" : [ null, null, null, null ],
  "secondaryFormationFractions" : [ [ null, null, null, null ], [ null, null, null, null ], [
null, null, null, null ], [ null, null, null, null ] ]
 },
 "applicationScheme" : {
  "applications" : [ ],
  "tcycle" : 1
 }
} ]
```


Tip: Use online JSON validators (f.i. https://jsonlint.com/, https://jsonformatter.org/, …) to validate your JSON file for being sure there are no commas or brackets forgotten.

13. Additional information

This section contains additional information such as:

- Crop Interception Factors
- Crop specification list
- EFSA Spatial version
- FOCUS Crops
- f_{ridge} and f_{furrow} for spray applications
- f_q, $f_{om,corr}$, z_{til}, $C_{T,ini}$ and $C_{T,plateau}$ in relation to crop and application type
- Scenario and model adjustment factors
- Soil specific parameters
- Wash-off fractions of the dose intercepted by Crop canopy
- Overview PERSAM input parameters

13.1. Crop Interception Factors[1]

CROP	FRACTION	GROWTHSTAGE
Apples (between crop in row, grass)	0,9	Jan-Mar
Apples (between crop in row, grass)	0,9	Apr-Jun
Apples (between crop in row, grass)	0,9	Jul-Sep
Apples (between crop in row, grass)	0,9	Oct-Dec
Bush berries (between crop in row, grass)	0,9	Jan-Mar
Bush berries (between crop in row, grass)	0,9	Apr-Jun
Bush berries (between crop in row, grass)	0,9	Jul-Sep
Bush berries (between crop in row, grass)	0,9	Oct-Dec
Citrus (between crop in row, bare soil)	0	Jan-Mar
Citrus (between crop in row, bare soil)	0	Apr-Jun
Citrus (between crop in row, bare soil)	0	Jul-Sep
Citrus (between crop in row, bare soil)	0	Oct-Dec
Hops (between crop in row, bare soil)	0	Jan-Mar
Hops (between crop in row, bare soil)	0	Apr-Jun
Hops (between crop in row, bare soil)	0	Jul-Sep
Hops (between crop in row, bare soil)	0	Oct-Dec
Olives (between crop in row, bare soil)	0	Jan-Mar
Olives (between crop in row, bare soil)	0	Apr-Jun
Olives (between crop in row, bare soil)	0	Jul-Sep
Olives (between crop in row, bare soil)	0	Oct-Dec
Vines (between crop in row, bare soil)	0	Jan-Mar
Vines (between crop in row, bare soil)	0	Apr-Jun
Vines (between crop in row, bare soil)	0	Jul-Sep
Vines (between crop in row, bare soil)	0	Oct-Dec
Apples (application on crop in row)	0,5	BBCH 0-9

[1] EFSA Guidance Document for evaluating laboratory and field dissipation studies to obtain DegT50 values of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal 2014;12(5):3662, 37 pp., doi:10.2903/j.efsa.2014.3662 – Appendix C table 1.4 & 1.5

CROP	FRACTION	GROWTHSTAGE
Apples (application on crop in row)	0,6	BBCH 10-69
Apples (application on crop in row)	0,65	BBCH 71-75
Apples (application on crop in row)	0,65	BBCH 76-89
Beans (field, veg.)	0	BBCH 0-9
Beans (field, veg.)	0,25	BBCH 10-19
Beans (field, veg.)	0,4	BBCH 20-39
Beans (field, veg.)	0,7	BBCH 40-89
Beans (field, veg.)	0,8	BBCH 90-99
Bush berries (application on crop in row)	0,4	BBCH 0-9
Bush berries (application on crop in row)	0,6	BBCH 10-69
Bush berries (application on crop in row)	0,75	BBCH 71-89
Cabbage	0	BBCH 0-9
Cabbage	0,25	BBCH 10-19
Cabbage	0,4	BBCH 20-39
Cabbage	0,7	BBCH 40-49
Cabbage	0,7	BBCH 50-89
Cabbage	0,9	BBCH 90-99
Carrots	0	BBCH 0-9
Carrots	0,25	BBCH 10-19
Carrots	0,6	BBCH 20-39
Carrots	0,8	BBCH 40-49
Carrots	0,8	BBCH 50-89
Carrots	0,8	BBCH 90-99
Citrus (application on crop in row)	0,8	Jan-Mar
Citrus (application on crop in row)	0,8	Apr-Jun
Citrus (application on crop in row)	0,8	Jul-Sep
Citrus (application on crop in row)	0,8	Oct-Dec
Cotton	0	BBCH 0-9

CROP	FRACTION	GROWTHSTAGE
Cotton	0,3	BBCH 10-19
Cotton	0,6	BBCH 20-39
Cotton	0,75	BBCH 40-89
Cotton	0,9	BBCH 90-99
Fallow	0	BBCH 0-99
Grass (pasture)	0,9	Jan-Mar
Grass (pasture)	0,9	Apr-Jun
Grass (pasture)	0,9	Jul-Sep
Grass (pasture)	0,9	Oct-Dec
Hops (application on crop in row)	0,4	BBCH 0-9
Hops (application on crop in row)	0,5	BBCH 11-13
Hops (application on crop in row)	0,6	BBCH 14-19
Hops (application on crop in row)	0,6	BBCH 20-52
Hops (application on crop in row)	0,6	BBCH 53-69
Hops (application on crop in row)	0,75	BBCH 71-89
Linseed	0	BBCH 0-9
Linseed	0,3	BBCH 10-19
Linseed	0,6	BBCH 20-39
Linseed	0,7	BBCH 40-89
Linseed	0,9	BBCH 90-99
Maize	0	BBCH 0-9
Maize	0,25	BBCH 10-19
Maize	0,5	BBCH 20-39
Maize	0,75	BBCH 40-89
Maize	0,9	BBCH 90-99
Oilseed rape (summer)	0	BBCH 0-9
Oilseed rape (summer)	0,4	BBCH 10-19
Oilseed rape (summer)	0,8	BBCH 20-39

CROP	FRACTION	GROWTHSTAGE
Oilseed rape (summer)	0,8	BBCH 40-89
Oilseed rape (summer)	0,9	BBCH 90-99
Oilseed rape (winter)	0	BBCH 0-9
Oilseed rape (winter)	0,4	BBCH 10-19
Oilseed rape (winter)	0,8	BBCH 20-39
Oilseed rape (winter)	0,8	BBCH 40-89
Oilseed rape (winter)	0,9	BBCH 90-99
Olives (application on crop in row)	0,7	Jan-Mar
Olives (application on crop in row)	0,7	Apr-Jun
Olives (application on crop in row)	0,7	Jul-Sep
Olives (application on crop in row)	0,7	Oct-Dec
Onions	0	BBCH 0-9
Onions	0,1	BBCH 10-19
Onions	0,25	BBCH 20-39
Onions	0,4	BBCH 40-49
Onions	0,4	BBCH 50-89
Onions	0,6	BBCH 90-99
Peas	0	BBCH 0-9
Peas	0,35	BBCH 10-19
Peas	0,55	BBCH 20-39
Peas	0,85	BBCH 40-89
Peas	0,85	BBCH 90-99
Potatoes	0	BBCH 0-9
Potatoes	0,15	BBCH 10-19
Potatoes	0,6	BBCH 20-39
Potatoes	0,85	BBCH 40-89
Potatoes	0,5	BBCH 90-99
Soybean	0	BBCH 0-9

CROP	FRACTION	GROWTHSTAGE
Soybean	0,35	BBCH 10-19
Soybean	0,55	BBCH 20-39
Soybean	0,85	BBCH 40-89
Soybean	0,65	BBCH 90-99
Spring cereals	0	BBCH 0-9
Spring cereals	0	BBCH 10-19
Spring cereals	0,2	BBCH 20-29
Spring cereals	0,8	BBCH 30-39
Spring cereals	0,9	BBCH 40-69
Spring cereals	0,8	BBCH 70-89
Spring cereals	0,8	BBCH 90-99
Strawberries	0	BBCH 0-9
Strawberries	0,3	BBCH 10-19
Strawberries	0,5	BBCH 20-39
Strawberries	0,6	BBCH 40-89
Strawberries	0,6	BBCH 90-99
Sugar beets	0	BBCH 0-9
Sugar beets	0,2	BBCH 10-19
Sugar beets	0,7	BBCH 20-39
Sugar beets	0,9	BBCH 40-49
Sugar beets	0,9	BBCH 50-89
Sugar beets	0,9	BBCH 90-99
Sunflowers	0	BBCH 0-9
Sunflowers	0,2	BBCH 10-19
Sunflowers	0,5	BBCH 20-39
Sunflowers	0,75	BBCH 40-89
Sunflowers	0,9	BBCH 90-99
Tobacco	0	BBCH 0-9

CROP	FRACTION	GROWTHSTAGE
Tobacco	0,5	BBCH 10-19
Tobacco	0,7	BBCH 20-39
Tobacco	0,9	BBCH 40-89
Tobacco	0,9	BBCH 90-99
Tomatoes	0	BBCH 0-9
Tomatoes	0,5	BBCH 10-19
Tomatoes	0,7	BBCH 20-39
Tomatoes	0,8	BBCH 40-89
Tomatoes	0,5	BBCH 90-99
Vines (application on crop in row)	0,4	BBCH 0-9
Vines (application on crop in row)	0,5	BBCH 11-13
Vines (application on crop in row)	0,6	BBCH 14-19
Vines (application on crop in row)	0,6	BBCH 53-69
Vines (application on crop in row)	0,75	BBCH 71-89
Winter cereals	0	BBCH 0-9
Winter cereals	0	BBCH 10-19
Winter cereals	0,2	BBCH 20-29
Winter cereals	0,8	BBCH 30-39
Winter cereals	0,9	BBCH 40-69
Winter cereals	0,8	BBCH 70-89
Winter cereals	0,8	BBCH 90-99

13.2. Crop specification list

Table 1: Crop specification with respect to crop naming, crop map, crop type, mechanical cultivation and precipitation + irrigation

Crop Nr.	FOCUS Crop	JRC crop map (CAPRI + FERA)	Crop type	Mechanical cultivation	Precipitation + irrigation (mm)[a]		
					North	Centre	South
01	Apples (between-row, grass)	APPLES	Permanent	No	No irr.	No irr.	No irr.
02	Apples (in-row)	APPLES	Permanent	No	No irr.	No irr.	1453
03	Beans (field, veg.)	PULSES	Annual	Not applicable	No irr.	910	No irr.
04	Bush berries (between-row, grass)	BUSHBERRIES	Permanent	No	No irr.	No irr.	No irr.
05	Bush berries (in-row)	BUSHBERRIES	Permanent	No	No irr.	900	1203
06	Cabbage	OTHER_VEGETABLES	Annual	Not applicable	No irr.	845	1072
07	Carrots	OTHER_VEGETABLES	Annual	Not applicable	No irr.	821	1075
08	Citrus (between-row, bare soil)	CITRUS	Permanent	Yes	No crop	No crop	No irr.
09	Citrus (in-row)	CITRUS	Permanent	No	No crop	No crop	1226
10	Cotton	TEXTURE_CROPS	Annual	Not applicable	No crop	No irr.	777
11	Fallow	FALLOW	Annual	Not applicable	No irr.	No irr.	No irr.
12	Grass (pasture)	GRASS	Permanent	No	No irr.	No irr.	No irr.
13	Hops (between-row, bare soil)	HOPS	Permanent	Yes	No crop	No irr.	No irr.
14	Hops (in-row)	HOPS	Permanent	No	No crop	No irr.	No irr.
15	Linseed	TEXTURE_CROPS	Annual	Not applicable	No irr.	No irr.	1172
16	Maize	MAIZE	Annual	Not applicable	No irr.	914	No irr.
17	Oilseed rape (summer)	RAPES	Annual	Not applicable	No irr.	No irr.	No irr.
18	Oilseed rape (winter)	RAPES	Annual	Not applicable	No irr.	No irr.	No irr.
19	Olives (between-row, bare soil)	OLIVES	Permanent	Yes	No crop	No crop	No irr.
20	Olives (in-row)	OLIVES	Permanent	Yes	No crop	No crop	1218
21	Onions	OTHER_VEGETABLES	Annual	Not applicable	No irr.	No irr.	675
22	Peas (animal)	PULSES	Annual	Not applicable	No irr.	No irr.	No irr.
23	Potatoes	POTATOES	Annual	Not applicable	No irr.	No irr.	No irr.
24	Soybean	SOYA	Annual	Not applicable	No crop	904	1033
25	Spring cereals	CEREALS_TOT[b]	Annual	Not applicable	No irr.	No irr.	No irr.
26	Strawberries	OTHER_VEGETABLES	Annual	Not applicable	No irr.	918	1119
27	Sugar beets	SUGARBEET	Annual	Not applicable	No irr.	No irr.	No irr.
28	Sunflowers	SUNFLOWER	Annual	Not applicable	No crop	1004	No irr.
29	Tobacco	TOBACCO	Annual	Not applicable	No crop	972	1233
30	Tomatoes	OTHER_VEGETABLES	Annual	Not applicable	No irr.	828	663
31	Vines (between-row, bare soil)	VINES	Permanent	Yes	No crop	No irr.	No irr.
32	Vines (in-row)	VINES	Permanent	No	No crop	887	1266
33	Winter cereals	CEREALS_TOT[b]	Annual	Not applicable	No irr.	No irr.	No irr.

(a) 'No irr.' indicates that a location specific precipitation is obtained from the EFSA spatial data set (as these locations are not irrigated)
(b) CEREALS_TOT includes the CAPRI crops barley, common wheat, durum wheat, oats, and rye

The order and number of crops in this list is binding (the crop number is part of the PERSAM transfer file).

13.3. EFSA Spatial data

The EFSA spatial data set version 1.1 includes following maps:

Table 1: EFSA Spatial data version 1.1

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

Mean monthly precipitation sum, April	EU27
Mean monthly precipitation sum, May	EU27
Mean monthly precipitation sum, June	EU27
Mean monthly precipitation sum, July	EU27
Mean monthly precipitation sum, August	EU27
Mean monthly precipitation sum, September	EU27
Mean monthly precipitation sum, October	EU27
Mean monthly precipitation sum, November	EU27
Mean monthly precipitation sum, December	EU27
Annual mean precipitation sum	EU27
Soil data	
Topsoil Organic Matter content	EU27
Topsoil pH	EU27
Topsoil Bulk Density	EU27
Topsoil Texture Class	EU27
Topsoil Water Content at Field Capacity	EU27
CAPRI2000 Crop Data	
EFSA-CAPRI Common Mask	EU25
EFSA-CAPRI Barley	EU25
EFSA-CAPRI Common wheat	EU25
EFSA-CAPRI Durum wheat	EU25
EFSA-CAPRI Fallow land	EU25
EFSA-CAPRI Floriculture	EU25
EFSA-CAPRI Maize	EU25
EFSA-CAPRI Oats	EU25
EFSA-CAPRI Other cereals	EU25
EFSA-CAPRI Other annual crops	EU25
EFSA-CAPRI Fodder other on arable land	EU25
EFSA-CAPRI Other non permanent industrial crops	EU25

EFSA-CAPRI Other root crops	EU25
EFSA-CAPRI Other fresh vegetables	EU25
EFSA_CAPRI Potatoes	EU25
EFSA-CAPRI Dry pulses	EU25
EFSA-CAPRI Rape and turnip rape	EU25
EFSA-CAPRI Rye	EU25
EFSA-CAPRI Soya	EU25
EFSA-CAPRI Sugar beet	EU25
EFSA-CAPRI Sunflower	EU25
EFSA-CAPRI Fibre and oleaginous crops	EU25
EFSA-CAPRI Tobacco	EU25
EFSA-CAPRI Tomatoes	EU25

EU25: E27 without Malta, Cyprus and some smaller areas

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

13.4. FOCUS Crops[2]

Table 1: Link between FOCUS and CAPRI crops for annual crops. The table further shows which FOCUS scenario (dominant FOCUS zone) is used to build the Tier-3A scenario

FOCUS crop	CAPRI crop[(d)]	North	Centre	South
Beans (field- and vegetable beans)[(c)]	Pulses	HA	CH	HA
Cabbage	Other fresh vegetables	HA	CH	SE
Carrots	Other fresh vegetables	HA	CH	SE
Cotton	Texture crops	–	HA	TH
Linseed	Texture crops	HA	HA	SE
Maize	Maize	HA	CH	HA
No crops (= fallow)	Fallow	HA	HA	SE
Oil seed rape (summer)	Oilseed rapes	HA	HA	HA
Oil seed rape (winter)	Oilseed rapes	HA	HA	HA
Onions[(a)]	Other fresh vegetables	HA	HA	SE
Peas (animal)	Pulses	HA	CH	HA
Potatoes	Potatoes	HA	HA	HA
Soybean	Soya beans	–	CH	TH
Spring cereals	Cereals[(b)]	HA	CH	HA
Strawberries	Other fresh vegetables	HA	CH	SE
Sugar beets	Sugar beets	HA	HA	HA
Sunflower	Sunflower	–	CH	HA
Tobacco	Tobacco	–	CH	TH
Tomatoes	Other fresh vegetables	HA	CH	SE
Winter cereals	Cereals[(b)]	HA	CH	HA

CH: Châteaudun; HA: Hamburg; JO: Jokioinen; KR: Kremsmünster; OK: Okehampton; PI: Piacenza; PO: Porto; SE: Seville; TH: Thiva. See EC (2014) for further details.
(a): Also to be used for flower bulbs because there is no such crop in FOCUS.
(b): Barley, common wheat, durum wheat, oats and rye.
(c): Field beans in North and Centre; vegetable beans in South.
(d): Used as a proxy of the area of potential use of the PPP.

[2] 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 2017;15(10):4982 doi: 10.2903/j.efsa.2017.4982

Table 2: Link between FOCUS crops and permanent crops. The table further shows which FOCUS scenario (dominant FOCUS zone) is used to build the Tier-3A scenario. Note that in permanent crops grown in rows there is a distinction between in-row and between-row exposure

FOCUS crop	Permanent crop[d]	North	Centre	South	Exposure type
Apples	Apples[e]	HA	HA	SE	In-row (apples)
					Between-row (grass cover)
Bush berries[a]	Bush berries	HA	CH	SE	In-row (bush berries)
					Between-row (grass cover)
Citrus	Citrus	–	–	SE	In-row (citrus)
					Between-row (bare soil)
Grass	Permanent grass	HA	HA	HA	Not relevant
Hops[b]	Hops	–	HA	HA	In-row (hops)
					Between-row (bare soil)
Olives[c]	Olives	–	–	SE	In-row (olives)
					Between-row (bare soil)
Vines	Vines	–	CH	SE	In-row (vines)
					Between-row (bare soil)

CH: Châteaudun; HA: Hamburg; JO: Jokioinen; KR: Kremsmünster; OK: Okehampton; PI: Piacenza; PO: Porto; SE: Seville. See EC (2014) for further details.

(a): Development stages set to those for FOCUS apples; all other crop parameters from FOCUS bush berries (Jokioinen only; Beulke et al., 2015).

(b): Not a FOCUS GW crop; citrus crop parameter used; max. Leaf Area Index (LAI) set to 5 m/m^3 (Beulke et al., 2015).

(c): Not a FOCUS GW crop; development stages, rooting depth and max. LAI taken from Beulke et al. (2015).

(d): Used as a proxy of the area of potential use of the PPP.

(e): Pome and stone fruits.

13.5. f_{ridge} and f_{furrow} for spray applications[3]

The following values are not implemented in PERSAM in case of potatoes. They have to be set manually.

Table 1: Values of f_{furrow} and f_{ridge} to be used for spray applications onto only the ridge or only the furrow

Regulatory zone	f_{ridge} (–)	f_{furrow} (–)
North	0.55	0.45
Centre	0.72	0.28
South	0.62	0.38

13.6. f_q, $f_{om,corr}$, z_{til}, $C_{T,ini}$ and $C_{T,plateau}$ in relation to crop and application type

Table 1: Annual crops: Soil organic matter correction factor ($f_{om,corr}$), reference depth for the leaching term (f_q), setting of the tillage depth (z_{til}) and calculation of the initial and plateau concentration ($C_{T,ini}$ and $C_{T,plateau}$) in PERSAM in relation to the application type

Application type	To the soil surface or crop canopy	Soil incorporation (Chapter 4.4.1 in the GD)	Placing at a certain soil depth (Chapter 4.4.2 in the GD)
Soil organic matter correction factor ($f_{om,corr}$) in PERSAM	= 1	= 1	= weighted average organic matter scaling factor from z_{inc} to $z_{inc} + z_{eco}$ (refer to Table D.3)
Reference depth for f_q	$= z_{eco}$	$= z_{eco}$	$= z_{inc} + z_{eco}$
z_{til} in PERSAM	= 20 cm	= 20 cm	$z_{inc} + z_{eco} < 20$ cm: = 20 cm $z_{inc} + z_{eco} \geq 20$ cm: $z_{inc} < 20$ cm: $= z_{inc} + z_{eco}$ $z_{inc} \geq 20$ cm: $= z_{eco}$
Initial concentration in PERSAM ($C_{T,ini}$)	Eqn. A1	$z_{inc} < z_{eco}$: Eqn. A1 $z_{inc} \geq z_{eco}$: Eqn. A19b	Eqn. A1
Plateau concentration in PERSAM ($C_{T,plateau}$)	Eqn. A2	$z_{inc} < 20$ cm: Eqn. A2 $z_{inc} \geq 20$ cm: Eqn. A19a	Eqn. A2

[3] EFSA (European Food Safety Authority), 2017. 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 2017;15(10):4982, 115 pp. https://doi.org/10.2903/j.efsa.2017.4982 - p 33 table 12

Table 2: Permanent crops: Soil organic matter correction factor ($f_{om,corr}$), reference depth for the leaching term (f_q), setting of the tillage depth (z_{til}) and calculation of the initial and plateau concentration ($C_{T,ini}$ and $C_{T,plateau}$) in PERSAM in relation to the application type

Application type	To the soil surface or crop canopy	Soil incorporation (Chapter 4.4.1 in the GD)	Placing at a certain soil depth (Chapter 4.4.2 in the GD)
Soil organic matter correction factor ($f_{om,corr}$) in PERSAM	= weighted average organic matter scaling factor from 0 to z_{eco} (refer to Table D.3)	= weighted average organic matter scaling factor from 0 to z_{eco}, (refer to Table D.3)	= weighted average organic matter scaling factor from z_{inc} to $z_{inc} + z_{eco}$ (refer to Table D.3)
Reference depth for f_q	$= z_{eco}$	$= z_{eco}$	$= z_{inc} + z_{eco}$
z_{til} in PERSAM	No mechanical cultivation: $= z_{eco}$ Mechanical cultivation: $z_{eco} < 5$ cm: $= 5$ cm; $z_{eco} \geq 5$ cm: $= z_{eco}$	No mechanical cultivation: $= z_{eco}$ Mechanical cultivation: $z_{eco} < 5$ cm: $= 5$ cm; $z_{eco} \geq 5$ cm: $= z_{eco}$	No mechanical cultivation: $= z_{eco}$ Mechanical cultivation: $z_{inc} + z_{eco} < 5$ cm: $= 5$ cm; $z_{inc} + z_{eco} \geq 5$ cm: $z_{inc} < 5$ cm: $= z_{inc} + z_{eco}$; $z_{inc} \geq 5$ cm: $= z_{eco}$
Initial concentration in PERSAM ($C_{T,ini}$)	Eqn. A1	$z_{inc} < z_{eco}$: Eqn. A1 $z_{inc} \geq z_{eco}$: Eqn. A19b	Eqn. A1
Plateau concentration in PERSAM ($C_{T,plateau}$)	Eqn. A2	No mechanical cultivation: $z_{inc} < z_{eco}$: Eqn. A2; $z_{inc} \geq z_{eco}$: Eqn. A19a Mechanical cultivation: $z_{inc} < 5$ cm: Eqn. A2; $z_{inc} \geq 5$ cm: $z_{inc} < z_{eco}$: Eqn. A2; $z_{inc} \geq z_{eco}$: Eqn. A19a	Eqn. A2

Table 3: Extended organic matter scaling factors depending on the application type, soil cultivation and the incorporation depth (z_{inc}) - numbers not explicitly mentioned in the GD are highlighted in yellow.

Soil depth (cm)	Annual crops (all types of application)	Permanent crops											
		Without mechanical cultivation						With mechanical cultivation					
		Application to the soil surface or crop canopy & Placing at a certain soil depth	Soil incorporation					Application to the soil surface or crop canopy & Placing at a certain soil depth	Soil incorporation				
			z_{inc} = 1 cm	z_{inc} = 5 cm	z_{inc} = 10 cm	z_{inc} = 20 cm	z_{inc} = 30 cm		z_{inc} = 1 cm	z_{inc} = 5 cm	z_{inc} = 10 cm	z_{inc} = 20 cm	z_{inc} = 30 cm
0-5	1.00	1.95	1.95	1.95	1.63	1.19	1.00	1.50	1.50	1.50	1.35	1.13	1.00
5-10	1.00	1.30	1.30	1.30	1.63	1.19	1.00	1.20	1.20	1.20	1.35	1.13	1.00
10-20	1.00	0.76	0.76	0.76	0.76	1.19	1.00	0.90	0.90	0.90	0.90	1.13	1.00
20-30	1.00	0.62	0.62	0.62	0.62	0.62	1.00	0.75	0.75	0.75	0.75	0.75	1.00
30-60	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50

13.7. Scenario and model adjustment factors [4]

Table 1: Minimum and maximum scenario adjustment factors for concentration in the total soil ($C_{T,peak}$) in annual crops based on the standards substances 1–19

CAPRI crop or crop group	z_{eco} 1 cm						z_{eco} 20 cm					
	North		Centre		South		North		Centre		South	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Cereals[(a)]	0.95	0.96	0.98	0.98	1.00	1.00	0.95	0.98	0.97	0.98	1.00	1.00
Fallow	1.01	1.01	1.00	1.01	0.98	0.98	1.01	1.02	0.99	1.01	0.93	0.98
Maize	0.72	0.75	0.88	0.91	0.99	0.99	0.63	0.75	0.73	0.91	0.95	0.99
Other fresh vegetables	0.97	0.98	0.93	0.95	0.93	0.95	0.97	0.98	0.82	0.95	0.74	0.95
Potatoes	0.93	0.93	1.01	1.01	1.03	1.04	0.93	0.96	0.99	1.01	1.03	1.06
Pulses	0.87	0.87	0.93	0.94	1.00	1.00	0.87	0.90	0.90	0.94	1.00	1.02
Rapes	0.93	0.93	0.93	0.94	1.02	1.03	0.93	0.95	0.93	0.97	1.02	1.05
Soya	NC	NC	0.84	0.87	0.83	0.86	NC	NC	0.64	0.87	0.53	0.86
Sugar beet	0.84	0.84	0.92	0.93	1.01	1.01	0.79	0.84	0.89	0.93	1.01	1.05
Sunflower	NC	NC	0.82	0.86	0.96	0.96	NC	NC	0.56	0.86	0.87	0.96
Texture crops	1.25	1.28	0.93	0.94	0.90	0.91	1.25	1.31	0.93	0.98	0.70	0.91
Tobacco	NC	NC	0.91	0.94	0.94	0.97	NC	NC	0.73	0.94	0.71	0.97

Max: maximum; Min: minimum; NC: no crop.
(a): Based on the combined crop area of barley, common wheat, durum wheat, oats and rye.

Table 2: Minimum and maximum scenario adjustment factors for the concentration in the liquid phase ($C_{L,peak}$) in annual crops based on the standards substances 1–19

CAPRI crop or crop group	z_{eco} 1 cm						z_{eco} 20 cm					
	North		Centre		South		North		Centre		South	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Cereals[(a)]	1.02	1.04	0.95	1.00	0.92	1.00	1.00	1.04	0.96	1.02	0.92	1.04
Fallow	1.02	1.04	0.95	1.03	1.00	1.06	1.00	1.04	0.95	1.03	1.00	1.07
Maize	1.00	1.02	1.03	1.17	0.85	0.95	0.99	1.02	0.80	1.17	0.85	1.00
Other fresh vegetables	1.00	1.00	1.02	1.05	1.08	1.15	0.97	1.01	0.84	1.05	0.75	1.15
Potatoes	1.00	1.00	0.95	1.02	0.92	1.06	0.97	1.08	0.96	1.02	0.92	1.06
Pulses	0.96	1.00	0.95	0.98	0.98	1.00	0.95	1.00	0.95	1.02	0.98	1.08
Rapes	1.02	1.04	0.92	0.96	0.79	0.90	1.02	1.05	0.91	1.01	0.79	0.97
Soya	NC	NC	1.03	1.24	0.85	0.98	NC	NC	0.82	1.24	0.71	0.98
Sugar beet	1.02	1.04	1.00	1.05	0.85	0.97	0.99	1.04	1.00	1.05	0.85	0.98
Sunflower	NC	NC	1.03	1.24	0.95	1.00	NC	NC	0.76	1.24	0.95	1.02
Texture crops	0.62	0.77	0.95	0.97	1.01	1.10	0.62	0.84	0.95	1.01	1.01	1.10
Tobacco	NC	NC	1.02	1.05	0.91	1.10	NC	NC	0.74	1.05	0.63	1.10

Max: maximum; Min: minimum; NC: no crop.
(a): Based on the combined crop area of barley, common wheat, durum wheat, oats and rye.

[4] EFSA (European Food Safety Authority), 2017. 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 2017;15(10):4982, 115 pp. https://doi.org/10.2903/j.efsa.2017.4982 - Appendix C tables 3.1 → 3.4/p 16 table 5/p 18 table 8

Table 3: Minimum and maximum scenario adjustment factors for concentration in the total soil (CT,peak) in permanent crops based on the standards substances 1–19

Permanent crop	z_{eco} 1 cm						z_{eco} 20 cm					
	North		Centre		South		North		Centre		South	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Apples – between row	0.78	0.80	0.86	0.90	0.88	0.95	0.83	0.86	0.87	0.93	0.87	0.96
Apples – in row	0.78	0.80	0.86	0.90	0.58	0.95	0.83	0.86	0.87	0.93	0.64	0.96
Berries – between row	0.86	0.88	1.01	1.06	0.79	0.89	0.89	0.92	0.97	1.02	0.79	0.92
Berries – in row	0.86	0.88	0.80	1.02	0.56	0.89	0.89	0.92	0.87	1.02	0.62	0.92
Citrus – between row	NC	NC	NC	NC	0.58	0.74	NC	NC	NC	NC	0.57	0.83
Citrus – in row	NC	NC	NC	NC	0.43	0.79	NC	NC	NC	NC	0.43	0.84
Hops – between row	NC	NC	0.68	0.77	0.94	0.98	NC	NC	0.83	0.89	1.05	1.11
Hops – in row	NC	NC	0.84	0.87	1.09	1.15	NC	NC	0.86	0.91	1.06	1.14
Olives – between row	NC	NC	NC	NC	0.54	0.76	NC	NC	NC	NC	0.58	0.85
Olives – in row	NC	NC	NC	NC	0.40	0.76	NC	NC	NC	NC	0.46	0.85
Permanent grass	0.97	0.97	1.10	1.17	1.16	1.24	0.98	0.99	1.07	1.14	1.13	1.35
Vines – between row	NC	NC	0.60	0.74	0.67	0.82	NC	NC	0.73	0.86	0.74	0.91
Vines – in row	NC	NC	0.59	0.83	0.55	0.89	NC	NC	0.67	0.88	0.60	0.92

Max: maximum; Min: minimum; NC: no crop.

Table 4: Minimum and maximum scenario adjustment factors for concentration in the liquid phase ($C_{L,peak}$) in permanent crops based on the standards substances 1–19

Permanent crop	z_{eco} 1 cm						z_{eco} 20 cm					
	North		Centre		South		North		Centre		South	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Apples – between row	0.97	1.04	1.00	1.05	1.04	1.13	1.01	1.11	0.97	1.04	1.03	1.09
Apples – in row	0.97	1.04	1.00	1.05	0.89	1.10	1.01	1.11	0.97	1.04	0.61	1.08
Berries – between row	0.98	1.04	0.85	0.96	0.98	1.12	1.02	1.12	0.84	0.99	0.93	1.17
Berries – in row	0.98	1.04	0.75	0.91	0.83	1.12	1.02	1.12	0.76	0.92	0.66	1.17
Citrus – between row	NC	NC	NC	NC	1.20	1.53	NC	NC	NC	NC	1.10	1.21
Citrus – in row	NC	NC	NC	NC	0.90	1.10	NC	NC	NC	NC	0.68	1.08
Hops – between row	NC	NC	1.04	1.13	0.80	0.87	NC	NC	0.92	1.00	0.67	0.91
Hops – in row	NC	NC	0.91	0.94	0.65	0.77	NC	NC	0.89	0.98	0.64	0.88
Olives – between row	NC	NC	NC	NC	1.26	1.56	NC	NC	NC	NC	1.08	1.29
Olives – in row	NC	NC	NC	NC	1.26	1.56	NC	NC	NC	NC	0.75	1.29
Permanent grass	0.91	0.96	0.67	0.78	0.73	0.86	0.92	0.98	0.64	0.80	0.70	0.93
Vines – between row	NC	NC	1.16	1.47	1.17	1.45	NC	NC	1.04	1.20	1.09	1.17
Vines – in row	NC	NC	0.93	1.17	0.90	1.09	NC	NC	0.80	1.14	0.67	1.08

Max: maximum; Min: minimum; NC: no crop.

Table 5: Default scenario adjustment factors (fs) used when performing an assessment for one of the predefined scenarios at Tier-1 for the three regulatory zones and for the concentration in total soil and for the concentration in pore water.

Regulatory zone	Default scenario adjustment factors to be used for the	
	Concentration in total soil	Concentration in pore water
North–Centre–South	1.4	1.6

Table 6: Model adjustment factors (fM) used when performing an assessment with the analytical model.

Zone	Model adjustment factors to be used for the	
	Concentration in total soil	Concentration in pore water
North–Centre–South	3.0	4.0

Table 7 Overview of inclusion of canopy processes, scenario adjustment factors, and model adjustment factors in the different modelling tiers of Figure 4. '+' indicates that the process or factor is included, '–' indicates that it is not included. Notice that the adjustment factors are automatically applied by the models

Tier	Canopy processes	Scenario adjustment factors	Model adjustment factors
1	–	+	+
2	+	–	+
3A	+	–	–
3B	+	–	–

13.8. Soil specific parameters [5]

Table 1: Properties of the predefined scenarios for annual crops and permanent crops used at Tier-1 for the concentration in total soil

Zone	Code	FOCUS zone	Member state	T_{arit} (a) (°C)	T_{arr} (b) (°C)	P (c) (mm)	f_{om} (d) (–)	Texture class	θ_{fc} (e) (m^3/m^3)	ρ (f) (kg/dm^3)
North	CTN	Hamburg	Estonia	5.7	7.6	639	0.220	Coarse	0.244	0.707
Centre	CTC	Hamburg	Poland	7.4	9.3	617	0.122	Coarse	0.244	0.934
South	CTS	Hamburg	France	10.2	11.7	667	0.070	Medium	0.349	1.117

Soil properties are those of the top 30 cm of the soil, for properties of the other soil layers refer to Appendix B.
CTC: scenario for the total concentration in the Centre Zone; CTN: scenario for the total concentration in the North Zone; CTS: scenario for the total concentration in the South Zone. Geographical coordinates of the scenarios are:
CTN – 5141/3991, CTC – 5281/3111, CTS – 3898/2932.
(a): T_{arit} is the arithmetic mean annual temperature.
(b): T_{arr} is the Arrhenius-weighted mean annual temperature (explained in EFSA PPR Panel, 2012).
(c): P is the annual mean precipitation (mm).
(d): f_{om} (–) is the organic-matter content averaged over the top 30 cm.
(e): θ_{fc} (m^3/m^3) is the water content at field capacity.
(f): ρ (kg/dm^3) is the dry bulk density of the soil.

[5] EFSA (European Food Safety Authority), 2017. 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 2017;15(10):4982, 115 pp. https://doi.org/10.2903/j.efsa.2017.4982 - p14/15 tables 1 → 3 / p54 table B.2

Table 2: Properties of the selected predefined scenarios for annual crops and permanent crops used at Tier-1 for the concentration in pore water

Zone	Code	FOCUS zone	Member state	T_{arit} [a] (°C)	T_{arr} [b] (°C)	P [c] (mm)	f_{om} [d] (–)	Texture class	θ_{fc} [e] (m^3/m^3)	ρ [f] (kg/dm^3)
North	CLN	Hamburg	Denmark	8.0	9.2	602	0.025	Medium	0.349	1.371
Centre	CLC	Châteaudun	Austria	9.3	11.3	589	0.018	Medium	0.349	1.432
South	CLS	Sevilla	Spain	15.4	16.7	526	0.010	Medium	0.349	1.521

Soil properties are those of the top 30 cm of the soil, for properties of the other soil layers refer to Appendix B.
CLC: scenario for the concentration in pore water for the Centre 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. Geographical coordinates of the scenarios are: CLN – 4422/3645, CLC – 4806/2872, CLS – 3490/1974.
(a): T_{arit} is the arithmetic mean annual temperature.
(b): T_{arr} is the Arrhenius-weighted mean annual temperature (explained in EFSA PPR Panel, 2012).
(c): P is the annual mean precipitation (mm).
(d): f_{om} (–) is the organic-matter content averaged over the top 30 cm.
(e): θ_{fc} (m^3/m^3) is the water content at field capacity.
(f): ρ (kg/dm^3) is the dry bulk density of the soil.

Table 3: Correction factors for estimating the distribution of organic matter within the top 30 cm of the soil in permanent crops. The organic-matter content of a layer is calculated by multiplying the correction factor below with the organic-matter content in Tables 1 and 2, respectively.

Depth (cm)	Correction factor for situations without mechanical cultivation (–)	Correction factor for situations with mechanical cultivation (–)
0–5	1.95	1.50
5–10	1.30	1.20
10–20	0.76	0.90
20–30	0.62	0.75

Table 4: Ratio (fq) of the mean annual water flux at different soil depths and the mean annual precipitation plus irrigation

1 cm	2.5 cm	5 cm	20 cm
0.80	0.75	0.70	0.50

13.9. Wash-off fractions of the dose intercepted by Crop canopy[6]

CROP	FRACTION	GROWTHSTAGE
Apples (application on crop in row)	0,55	BBCH 0-9
Apples (application on crop in row)	0,6	BBCH 10-69
Apples (application on crop in row)	0,6	BBCH 71-75
Apples (application on crop in row)	0,55	BBCH 76-89
Beans (field, veg.)	0	BBCH 0-9
Beans (field, veg.)	0,6	BBCH 10-19
Beans (field, veg.)	0,75	BBCH 20-39

[6] EFSA (European Food Safety Authority), 2017. 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 2017;15(10):4982, 115 pp. https://doi.org/10.2903/j.efsa.2017.4982 - p 20/21 tables 9 & 10

CROP	FRACTION	GROWTHSTAGE
Beans (field, veg.)	0,8	BBCH 40-89
Beans (field, veg.)	0,35	BBCH 90-99
Bush berries (application on crop in row)	0,5	BBCH 0-9
Bush berries (application on crop in row)	0,6	BBCH 10-69
Bush berries (application on crop in row)	0,55	BBCH 71-89
Cabbage	0	BBCH 0-9
Cabbage	0,6	BBCH 10-19
Cabbage	0,8	BBCH 20-39
Cabbage	0,4	BBCH 40-49
Cabbage	0	BBCH 50-89
Cabbage	0	BBCH 90-99
Carrots	0	BBCH 0-9
Carrots	0,75	BBCH 10-19
Carrots	0,85	BBCH 20-39
Carrots	0,5	BBCH 40-49
Carrots	0	BBCH 50-89
Carrots	0	BBCH 90-99
Cotton	0	BBCH 0-9
Cotton	0,65	BBCH 10-19
Cotton	0,75	BBCH 20-39
Cotton	0,65	BBCH 40-89
Cotton	0,45	BBCH 90-99
Fallow	0	BBCH 0-99
Hops (application on crop in row)	0,5	BBCH 0-9
Hops (application on crop in row)	0,55	BBCH 11-13
Hops (application on crop in row)	0,55	BBCH 14-19
Hops (application on crop in row)	0,55	BBCH 20-52
Hops (application on crop in row)	0,55	BBCH 53-69
Hops (application on crop in row)	0,6	BBCH 71-89
Linseed	0	BBCH 0-9
Linseed	0,55	BBCH 10-19
Linseed	0,75	BBCH 20-39
Linseed	0,6	BBCH 40-89
Linseed	0,3	BBCH 90-99
Maize	0	BBCH 0-9
Maize	0,45	BBCH 10-19
Maize	0,65	BBCH 20-39

CROP	FRACTION	GROWTHSTAGE
Maize	0,7	BBCH 40-89
Maize	0,55	BBCH 90-99
Oilseed rape (summer)	0	BBCH 0-9
Oilseed rape (summer)	0,4	BBCH 10-19
Oilseed rape (summer)	0,5	BBCH 20-39
Oilseed rape (summer)	0,6	BBCH 40-89
Oilseed rape (summer)	0,5	BBCH 90-99
Oilseed rape (winter)	0	BBCH 0-9
Oilseed rape (winter)	0,1	BBCH 10-19
Oilseed rape (winter)	0,4	BBCH 20-39
Oilseed rape (winter)	0,55	BBCH 40-89
Oilseed rape (winter)	0,3	BBCH 90-99
Onions	0	BBCH 0-9
Onions	0,6	BBCH 10-19
Onions	0,75	BBCH 20-39
Onions	0,55	BBCH 40-49
Onions	0	BBCH 50-89
Onions	0	BBCH 90-99
Peas	0	BBCH 0-9
Peas	0,4	BBCH 10-19
Peas	0,6	BBCH 20-39
Peas	0,65	BBCH 40-89
Peas	0,35	BBCH 90-99
Potatoes	0	BBCH 0-9
Potatoes	0,3	BBCH 10-19
Potatoes	0,5	BBCH 20-39
Potatoes	0,6	BBCH 40-89
Potatoes	0,35	BBCH 90-99
Soybean	0	BBCH 0-9
Soybean	0,55	BBCH 10-19
Soybean	0,75	BBCH 20-39
Soybean	0,8	BBCH 40-89
Soybean	0,35	BBCH 90-99
Spring cereals	0	BBCH 0-9
Spring cereals	0,4	BBCH 10-19
Spring cereals	0,5	BBCH 20-29
Spring cereals	0,5	BBCH 30-39

CROP	FRACTION	GROWTHSTAGE
Spring cereals	0,65	BBCH 40-69
Spring cereals	0,65	BBCH 70-89
Spring cereals	0,55	BBCH 90-99
Strawberries	0	BBCH 0-9
Strawberries	0,5	BBCH 10-19
Strawberries	0,7	BBCH 20-39
Strawberries	0,75	BBCH 40-89
Strawberries	0,5	BBCH 90-99
Sugar beets	0	BBCH 0-9
Sugar beets	0,4	BBCH 10-19
Sugar beets	0,6	BBCH 20-39
Sugar beets	0,6	BBCH 40-49
Sugar beets	0	BBCH 50-89
Sugar beets	0	BBCH 90-99
Sunflowers	0	BBCH 0-9
Sunflowers	0,6	BBCH 10-19
Sunflowers	0,75	BBCH 20-39
Sunflowers	0,8	BBCH 40-89
Sunflowers	0,55	BBCH 90-99
Tobacco	0	BBCH 0-9
Tobacco	0,55	BBCH 10-19
Tobacco	0,75	BBCH 20-39
Tobacco	0,8	BBCH 40-89
Tobacco	0,85	BBCH 90-99
Tomatoes	0	BBCH 0-9
Tomatoes	0,55	BBCH 10-19
Tomatoes	0,75	BBCH 20-39
Tomatoes	0,7	BBCH 40-89
Tomatoes	0,35	BBCH 90-99
Vines (application on crop in row)	0,45	BBCH 0-9
Vines (application on crop in row)	0,4	BBCH 11-13
Vines (application on crop in row)	0,5	BBCH 14-19
Vines (application on crop in row)	0,55	BBCH 53-69
Vines (application on crop in row)	0,6	BBCH 71-89
Winter cereals	0	BBCH 0-9
Winter cereals	0,1	BBCH 10-19
Winter cereals	0,4	BBCH 20-29

CROP	FRACTION	GROWTHSTAGE
Winter cereals	0,6	BBCH 30-39
Winter cereals	0,55	BBCH 40-69
Winter cereals	0,6	BBCH 70-89
Winter cereals	0,4	BBCH 90-99
Apples (between crop in row, grass)	0,45	Jan-Mar
Apples (between crop in row, grass)	0,55	Apr-Jun
Apples (between crop in row, grass)	0,55	Jul-Sep
Apples (between crop in row, grass)	0,5	Oct-Dec
Bush berries (between crop in row, grass)	0,45	Jan-Mar
Bush berries (between crop in row, grass)	0,55	Apr-Jun
Bush berries (between crop in row, grass)	0,55	Jul-Sep
Bush berries (between crop in row, grass)	0,5	Oct-Dec
Citrus (between crop in row, bare soil)	0	Jan-Mar
Citrus (between crop in row, bare soil)	0	Apr-Jun
Citrus (between crop in row, bare soil)	0	Jul-Sep
Citrus (between crop in row, bare soil)	0	Oct-Dec
Hops (between crop in row, bare soil)	0	Jan-Mar
Hops (between crop in row, bare soil)	0	Apr-Jun
Hops (between crop in row, bare soil)	0	Jul-Sep
Hops (between crop in row, bare soil)	0	Oct-Dec
Olives (between crop in row, bare soil)	0	Jan-Mar
Olives (between crop in row, bare soil)	0	Apr-Jun
Olives (between crop in row, bare soil)	0	Jul-Sep
Olives (between crop in row, bare soil)	0	Oct-Dec
Vines (between crop in row, bare soil)	0	Jan-Mar
Vines (between crop in row, bare soil)	0	Apr-Jun
Vines (between crop in row, bare soil)	0	Jul-Sep
Vines (between crop in row, bare soil)	0	Oct-Dec
Citrus (application on crop in row)	0,5	Jan-Mar
Citrus (application on crop in row)	0,3	Apr-Jun
Citrus (application on crop in row)	0,15	Jul-Sep
Citrus (application on crop in row)	0,55	Oct-Dec
Olives (application on crop in row)	0,5	Jan-Mar
Olives (application on crop in row)	0,3	Apr-Jun
Olives (application on crop in row)	0,15	Jul-Sep
Olives (application on crop in row)	0,5	Oct-Dec
Grass (pasture)	0,45	Jan-Mar

CROP	FRACTION	GROWTHSTAGE
Grass (pasture)	0,55	Apr-Jun
Grass (pasture)	0,55	Jul-Sep
Grass (pasture)	0,5	Oct-Dec

13.10. Overview PERSAM input parameters

These are the required user provided input data. All other input data is built-in in lookup tables and/or spatial data.

Annual application rate

symbol	unit	description	origin
n		number of applications	user provided
A_i	kg/ha	application rate of application i	user provided
$t_{app,i}$	day index	day-of-year of application i	user provided
$BBCH_i$		code (0-99) characterizing the crop development stage at application i	user provided
m		number of metabolite formation pathways	user provided
M_{met}	g/mol	Molar mass of the metabolite considered (primary or secondary)	user provided
M_{parent}	g/mol	Molar mass of the parent substance	user provided
$F_{f,p,j}$		formation fraction of the primary metabolite	user provided
$F_{f,s,j}$		formation fraction of the secondary metabolite	user provided

Simple analytical model

symbol	unit	description	origin
A_{year}	kg/ha ≈ mg/dm^2	annual application rate	calculated
t_{cycle}	days	time between applications (365, 730, or 1095 days)	user provided
E	kJ/mol	Arrhenius activation energy	user provided
$DegT_{50}$	days	degradation half-life in soil at reference temperature	user provided
K_{om}	ml/g	coefficient for sorption on organic matter	user provided
z_{inc}	dm	incorporation depth (optional)	user provided
z_{eco}	dm	ecotoxicological averaging depth	user selected value out of list of fixed values
tavg	days	time period since application time over which concentrations are averaged	user selected value out of list of fixed values

symbol	unit	description	origin
		Tier-1: crop type (annual or permanent)	user provided
		Tier-2/Tier-3A: FOCUS crop	user provided
		endpoints (concentration in total soil and/or concentration in liquid phase)	user provided
		regulatory zones (north, central, and/or south)	user provided

13.11. PERSAM 3 export/import file format

The PERSAM 3 export/import file format is a plain text file containing a list of PERSAM projects in JSON format. We will refer to this file format as the 'export file format' further on in this document.

13.11.1. JSON

For in depth information about the JSON format itself, please refer to

https://json.org/

https://en.wikipedia.org/wiki/JSON

An example of a JSON (syntax) validator:

https://duck.co/ia/view/json_validator

13.11.2. Valid export files

An export file reflects a list of PERSAM project configurations. When using the PERSAM GUI, the user can only create valid project configurations. The GUI does not allow invalid configuration settings. Therefore, the export files generated by PERSAM itself will always be valid export files.

Since the export file format is a plain text format, the user can easily create these files using external tools. Export files can be created by scripting/programming or by hand in a text editor.

When importing export files, PERSAM will not validate those files. However, if the project configuration is not valid, things will go horribly wrong when running the calculations. Unexpected error dialogs will be shown in those cases.

So please make sure you create valid export files before importing them into PERSAM. This document only describes the export file format. That is: all possible content of the export files. Not all possible combinations of this content are valid project configurations. Valid project configurations are described in the EFSA guidance document, and are implemented in the PERSAM GUI. You can use these 2 as sources of documentation on how to create valid project configurations.

Files that have a valid JSON syntax are not automatically valid export files. All examples below have a valid JSON syntax, but are invalid export files. You can use the PERSAM GUI to create examples of valid export files.

Note that export files are case sensitive: "belgium" is a different value than "Belgium".

13.11.3. High level export file structure

The main element in the export file is a list of (project) objects. A list in JSON is surrounded by []. An object in JSON is surrounded by {}. Items in a list in JSON are separated by a ,. An export file containing 2 empty projects looks as follows.

```
[ {}, {} ]
```

Note that this is an invalid export file: projects cannot be empty.

13.11.4. Project fields

A project contains up to 7 fields: name, description, outputFolder, properties, settings, substanceTree, and applicationScheme. The name, description, and outputFolder fields are text typed fields. The properties, settings, substanceTree, and applicationScheme are object typed fields.

For example:

```
[ {
        "name" : "example project",
        "outputFolder" : "C:\example\output\folder",
        "properties" : {},
        "settings" : {},
        "substanceTree" : {},
        "applicationScheme" : {}
} ]
```

Note:

. The description field is missing. This means it is empty. Empty fields do not have to be explicitly defined as empty: they can be left out.

. This is also an invalid export file: properties, settings, substanceTree, and applicationScheme cannot be empty objects.

13.11.5. The properties object

The properties object contains up to 9 fields: tier, substanceType, regionType, regions, cropType, crop, customCropMap, endpoints, and applicationType.

tier is a text typed field. Valid values are: tier1, tier2 (When tier2 is selected, tier3a will be calculated as well)

substanceType is a text typed field. Valid values are: microbialActive, other

regionType is a text typed field. Valid values are: zone, euMemberState

regions is a list typed field of text typed values. Valid list item values are: north, central, south, Austria, Belgium, Bulgaria, Cyprus, CzechRepublic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Poland, Portugal, Romania, Slovakia, Slovenia, Spain, Sweden, UnitedKingdom

cropType is a text typed field. Valid values are: permanent, annual

crop is a text typed field. Valid values are: apples, applesInRow, beans, bushBerries, bushBerriesInRow, cabbage, carrots, citrus, citrusInRow, cotton, fallow, grass, hops, hopsInRow, linseed, maize, oilseedRapeSummer, oilseedRapeWinter, olives, olivesInRow, onions, peas, potatoes, soybean, springCereals, strawberries, sugarBeets, sunflowers, tobacco, tomatoes, vines, vinesInRow, winterCereals

customCropMap is a text typed field containing the full path name of the file containing the (optional) custom crop map to use.

endpoints is a list typed field of text typed values. Valid list item values are: totalSoil, poreWater

applicationType is a text typed field. Valid values are: soilSurface, cropCanopy, soilDepth, soilIncorporation

For example:

```
"properties" : {
   "tier" : "tier3A",
   "substanceType" : "other",
   "regionType" : "zone",
   "regions" : [ "north", "central", "south" ],
   "cropType" : "annual",
   "crop" : "cabbage",
   "endpoints" : [ "totalSoil", "poreWater" ],
   "applicationType" : "soilSurface"
}
```

13.11.6. The settings object

The settings object contains up to 9 fields: tavg, tpostApp, zinc, ftreated, zecoTotalSoil, zecoPoreWater, racTotalSoil, racPoreWater, and exportGeneratedMaps.

tavg and tpostApp are number typed fields containing an integer value.

zinc, ftreated, zecoTotalSoil, zecoPoreWater are number typed fields containing a floating point value.

exportGeneratedMaps is a boolean typed field. Valid values are: true, false

For example:

```
"settings" : {
   "exportGeneratedMaps" : false,
   "ftreated" : 1.0,
   "zecoTotalSoil" : 1.0,
   "zecoPoreWater" : 20.0
}
```

13.11.7. The substanceTree object

The substanceTree object contains 5 fields: parentSubstance, primaryMetabolites, secondaryMetabolites, primaryFormationFractions, and secondaryFormationFractions.

parentSubstance is an object typed field containing a substance object defining the parent substance.

primaryMetabolites is a list typed field of substance objects defining the 4 primary metabolites, which may be empty.

secondaryMetabolites is a list typed field of substance objects defining the 4 secondary metabolites, which may be empty.

primaryFormationFractions is a list typed field of number typed values defining the formation fractions between the parent substance and the primary metabolites.

secondaryFormationFractions is a list typed field of list typed values of number typed values defining the formation fractions between the primary metabolites and the secondary metabolites. The first list in the list contains the formation fractions between the first primary metabolite and the secondary metabolites. The second list in the list contains the formation fractions between the second primary metabolite and the secondary metabolites. And so on.

A substance object contains up to 18 fields: substanceDefinition, code, kom, degT50, m, e, racTotalSoil, racPoreWater, komEquation, komMinimum, komMaximum, pka, deltaPh, manion, macid, komAnion, komAcid, degT50Equation, degT50Minimum, and degT50Maximum.

substanceDefinition is a text typed field. Valid values are: predefined1, predefined2, predefined3, predefined4, predefined5, predefined6, predefined7, predefined8, predefined9, predefined10, predefined11, predefined12, predefined13, predefined14, predefined15, predefined16, predefined17, predefined18, predefined19, custom

code is a text typed field.

kom, degT50, m and e are number typed fields containing floating point values.

komEquation is a text typed field.

komMinimum, komMaximum, pka, deltaPh, manion, macid, komAnion, komAcid are number typed fields containing floating point values.

degT50Equation is a text typed field.

degT50Minimum and degT50Maximum are number typed fields containing floating point values.

For example:


```
"substanceTree" : {
  "parentSubstance" : {
    "substanceDefinition" : "predefined1",
    "code" : "standard substance 1",
    "kom" : 10.0,
    "degT50" : 10.0,
    "m" : 300.0,
    "e" : 65.4,
   "racTotalSoil" : 8.0,
   "racPoreWater" : 0.6
  },
  "primaryMetabolites" : [ {
    "substanceDefinition" : "custom",
    "code" : "custom substance",
    "m" : 300.0,
    "e" : 65.4,
    "deltaPh" : 3.0,
    "komAnion" : 4785.0,
    "komAcid" : 36.5,
    "degT50Equation" : "om  *  log( ph )",
    "degT50Minimum" : 25.0,
    "degT50Maximum" : 106.0,
    "macid" : 106.0,
```

```
      "manion" : 102.0,
      "pka" : 25.0
    }, { }, {
      "substanceDefinition" : "predefined6",
      "code" : "standard substance 6",
      "kom" : 100.0,
      "degT50" : 10.0,
      "m" : 300.0,
      "e" : 65.4
    }, { } ],
    "secondaryMetabolites" : [ { }, {
      "substanceDefinition" : "predefined18",
      "code" : "standard substance 18",
      "kom" : 1000.0,
      "degT50" : 316.0,
      "m" : 300.0,
      "e" : 65.4
    }, { }, { } ],
    "primaryFormationFractions" : [ 0.63, null, 0.25, null ],
    "secondaryFormationFractions" : [ [ null, null, null, null ], [ null, null, null, null ], [ null, 0.05, null, null ], [ null, null, null, null ] ]
  }
```


13.11.8. The applicationScheme object

The applicationScheme object contains up to 3 fields: applications, simpleApplications, and tcycle.

applications is a list typed field of application objects.

simpleApplications is a list typed field of number values containing floating point values, which define the application doses for each application of microbial active substances.

tcycle is a number typed field containing an integer value. (1, 2, or 3)

An application object contains 3 fields: applicationRate, dayIndex, and growthStage.

applicationRate is a number typed field containing a floating point value.

dayIndex is a number typed field containing an integer value.

growthStage is a text typed field.

For example:


```
  "applicationScheme" : {
    "applications" : [ {
      "applicationRate" : 1.0,
```

```
      "dayIndex" : 0,
      "growthStage" : "BBCH 0-9"
    } ],
    "tcycle" : 1
}
```


References

European Food Safety Authority, 2014. EFSA Guidance Document for evaluating laboratory and field dissipation studies to obtain DegT50 values of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal 2014;12(5):3662, 37 pp., doi:10.2903/j.efsa.2014.3662

EFSA (European Food Safety Authority), 2017. 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 2017;15(10):4982, 115 pp. https://doi.org/10.2903/j.efsa.2017.4982

Tender specifications 'Update of PERSAM software models for predicting environmental concentrations of plant protection products in soil in permanent crop and annual crops.', reference: OC/EFSA/PRAS/2018/01

Abbreviations

CAPRI	Common Agricultural Policy Regionalised Impact model
CFD	Cumulative frequency distribution
C_L	Liquid concentration in soil ($mg.L^{-1}$)
C_T	Total concentration in soil ($mg.kg^{-1}$)
$DegT_{50}$	Degradation half-life in soil (days)
ρ	Dry bulk density of the soil ($kg.dm^{-3}$)
E	Arrhenius activation energy
f_M	Model adjustment factors
f_{om}	Organic matter content (-)
f_S	Default scenario adjustment factors
f_{soil}	Fraction that reaches the soil (-)
K_{om}	Organic matter/water distribution coefficient ($L.kg^{-1}$)
M	Molar mass
R	Gas constant
RAC	Regulatory Acceptable Concentration. RAC in total soil: mg/kg, RAC in pore water: mg/L
T_{arit}	Arithmetic mean temperature (K)
T_{arr}	Arrhenius weighted average soil temperature (K)
t_{avg}	Averaging time
t_{cycle}	Time between applications
$t_{postapp}$	Post-harvest interval. Interval between the last application and harvest.
T_{ref}	Reference temperature
θ_{fc}	Water content at field capacity ($m^3.m^{-3}$)
z_{eco}	Ecotoxicological averaging depth
z_{til}	Plough depth