EXTERNAL SCIENTIFIC REPORT

Software tool for calculating the predicted environmental concentrations of Plant Protection Products in soil[1]

PERSAM

CFT/EFSA/PRAS/2012/03

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

VITO

ABSTRACT

PERSAM is a software tool for calculating the predicted environmental concentrations of substances and their transformation products in soil in support of the EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. The tool is based on an analytical model for which both the concepts and the mathematical equations are described in the Scientific Opinion, (EFSA, 2012b). The software application assist the user in performing calculations using the analytic model, as described in the opinion. The PERSAM tool can be used to derive PECs in soil for spray applications to annual crops for conventional and reduced tillage.

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KEY WORDS

exposure assessment, soil, plant protection products, soil organisms, ecotoxicological effects, tiered approaches

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SUMMARY

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

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

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

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

The project started in December 2012 and was finalised in April 2014. This document describes the project approach, the implementation (high level) and the project results.

The PERSAM tool can be used to derive PECs in soil for spray applications to annual crops for conventional and reduced tillage.

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BACKGROUND AS PROVIDED BY EFSA

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

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

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

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

TERMS OF REFERENCE AS PROVIDED BY EFSA

This contract was awarded by EFSA to:

VITO

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

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

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INTRODUCTION AND OBJECTIVES

1. INTRODUCTION

The aims and objectives of the project are to develop a software tool for calculating the predicted environmental concentrations of substances and their transformation products in soil in support of the EFSA guidance document for predicting environmental concentrations of PPP's in soil. The tool shall be based on an analytical model for which both the concepts and the mathematical equations are described in the Scientific Opinion (EFSA, 2012b).

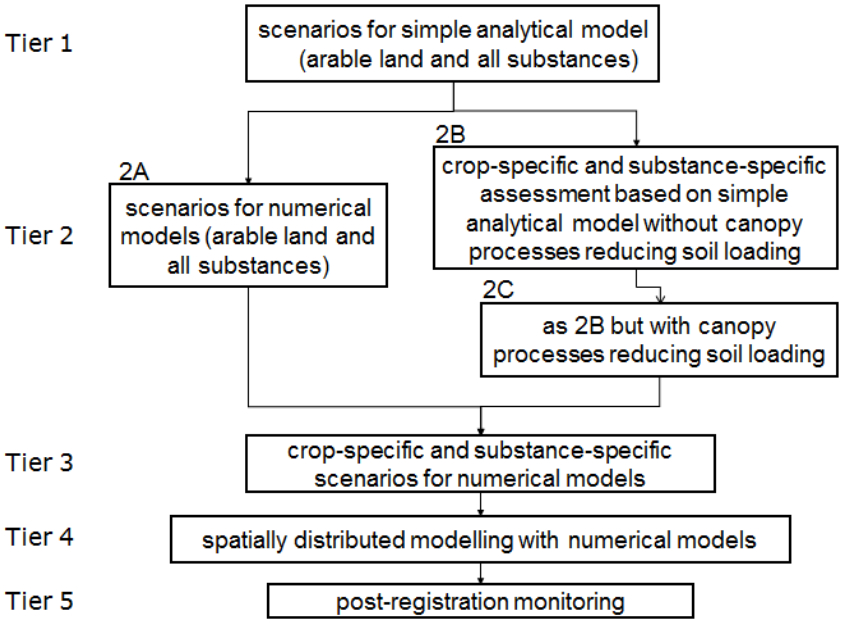

Figure 1: Outline of the different tiers in the exposure assessment of spray applications to annual crops for conventional and reduced tillage

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

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

The PERSAM tool and the PERSAM user manual can be downloaded freely on the JRC soil portal (*http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/).* The PERSAM user manual can also be downloaded on the EFSA website (*http://www.efsa.europa.eu/*) .

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2. GENERAL OBJECTIVES

The general objectives in this project are:

- ✓ *The software application must be conform to the requirements described in the EFSA Opinion on the science for scenario selection and scenario parameterization for predicting environmental concentrations of plant protection products in soil.*
- ✓ *The software should be user-friendly allowing applicants and risk assessors to perform the calculations.*
- ✓ *The user should be able to print the results of the statistical analysis and have access to the standard printing options available in screens applications*
- ✓ *The user should be able to save the results of the statistical analysis in .pdf and csv-format*
- ✓ *The reporting format should be conform to the EFSA requirements for the reporting of statistical analysis of field trial results, and should be suitable for inclusion in the dossier for regulatory purposes*
- ✓ *Installation of the software tool will not require additional software tools or applications* [2]
- ✓ *The tool should be a stand-alone application for installation on the local computer of the user and available for download from the EFSA website and shall run on Windows XP, window 7 and Windows 8. Previous versions of Windows are not supported by Microsoft therefore we cannot guarantee that the software application will run on these versions.*
- ✓ *The software application can be installed on a server (version Windows 2008 or higher) so that users can use the application using f.i. remote desktop VNC software.*
- ✓ *The application should be freely downloadable from the given website*
- ✓ *The software tool should be able to store the user defined input- and outputs, so that the user of the tool can reproduce or change the calculation regarding these user defined parameters when this is necessary.*
- ✓ *The tool should be able to generate a report (by export to pdf and to ESRI ASCII files) that can be submitted to registration authorities. The software should allow users to reset analysis options to system defaults. The users should be able to copy and paste text from the pdf report to word. The export to ESRI ASCII files is optional and by default unchecked since the generation of these files requires a lot of disk space (see Table 3).*
- ✓ *The software tool should be flexible enough to enable further modules to be added in the future (for example to accommodate calculations for scenarios for permanent crops that may be developed in the future).*
- ✓ *The software tool should correctly describe the 95th percentile PECs for all Tiers and scenario properties for Tier 3.*
- ✓ *The software uses the maps from the Joint Research Centre (JRC) website*[3]
- ✓ *The source code and scenario properties used by the model should be protected against modifications by the user.*
- ✓ *The use of the software tool should be described in a manual.*
- ✓ *A context sensitive help file should be provided to assist easy comprehension.*

[2] This is explained in more detail in section3.2.1 of the draft technical report 'Software tool for calculating the predicted environmental concentrations (PEC) of plant protection products (PPP) in soil : Software architecture'

[3] See http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/

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MATERIALS AND METHODS

1. PROJECT APPROACH

1.1. Project structure and management

The project structure and management consists of following roles:

Table 1: Project structure and management

	Description	Project team
Role		
Sponsor	EFSA is the sponsor for the development of the software tool PERSAM and is responsible with the EFSA WG PECs in soil for the validation and the acceptance of the software tool to guarantee the quality of the calculated results.	EFSA WG PECs in soil
VITO project manager	The project manager is responsible for the management of the project, the team, the communication and the interactions with EFSA. An important aspect is the notification of critical risks (timing, scope, objectives, …) and proposing mitigation strategies.	Jan Bronders
VITO business analyst	The business analyst interacts between functional (users, scientists, …) and technical groups (ICT) and is responsible for performing the functional analysis, the preparation of the project plan, the preparation of a test plan and so on.	Lieve Decorte
VITO model expert	The model expert has the expertise in environmental fate modeling in order to support the whole project	Ingeborg Joris
VITO IT experts	The IT experts are responsible for designing, developing and testing the software application.	Stijn Van Looy Wim Peelaerts

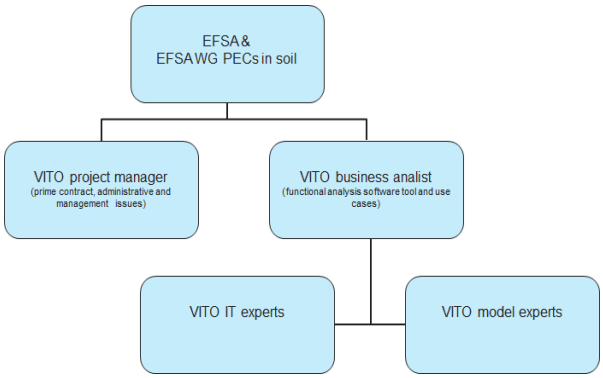

Figure 2: Project structure and management

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1.2. Project roadmap

Figure 4 shows the project roadmap containing 6 phases: the functional analysis, the technical analysis, implementation cycle 1, implementation cycle 2, implementation cycle 3 and preparation for launch & D-day (Delivery day)[4].

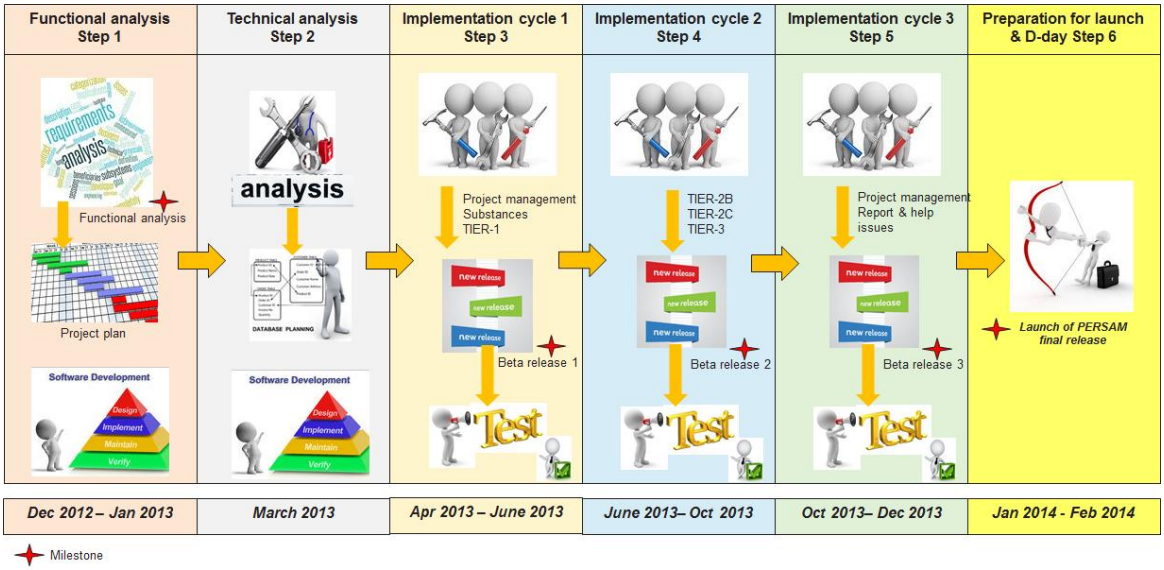

Figure 3: Project roadmap

The roadmap contains five milestones, indicated by ✦.

- ✓ Milestone 1: Delivery of the functional analysis
- ✓ Milestone 2: Delivery of beta release version 1
- ✓ Milestone 3: Delivery of beta release version 2
- ✓ Milestone 4: Delivery of beta release version 3
- ✓ Milestone 5: Delivery of the final release

1.2.1. Phase 1: Functional analysis

The functional analysis of the software application describes in detail the different functionalities based on user requirements and use cases. There are 7 use cases defined:

- ✓ Project
- ✓ Substances
- ✓ TIER-1
- ✓ TIER-2B
- ✓ TIER-2C
- ✓ TIER-3
- ✓ Report

[4] D-day is the day of the final release of PERSAM.

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Every use case is illustrated with mock-up screens for a better understanding of the functionalities.

The functional analysis is UML (*Unified Modelling Language*) based and contains different diagrams whereby every diagram contains more detailed information and is based on the previous part. Figure 5 shows the different parts.

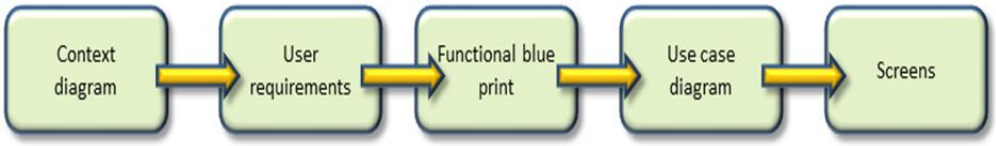

Figure 4: Different parts in the functional analysis

Context diagram

The Context diagram shows the system under consideration as a single high-level process and then shows the existing relationships between the system and other external entities (systems, organizational groups, external data stores, etc.).

User requirements

User requirements describe the tasks that users must perform when using the new product or system.

Functional blue print

The functional blue print is a business process diagram that shows in a hierarchical way a functional decomposition of the different processes on which the application is based. The business process at the basis of this hierarchy is called the primary business process and carries the name of the application itself and secondary business processes are coupled on this corresponding to the central concepts or objects of the application. A last division shows the different operations that can be carried out with the concepts or objects. A business process diagram generally contains three to four hierarchical levels. Each elementary business process forms the basis for a use case diagram.

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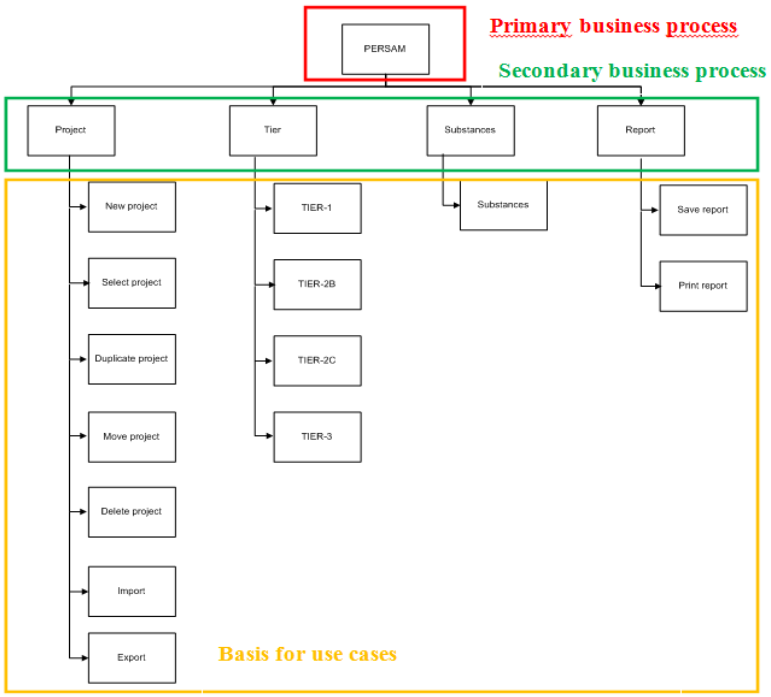

Figure 5: General functional blue print

Use case diagram

A use case diagram describes the functional requirements of a system using use cases and actors. This model is used to communicate with end users and ensures that the user requirements for the software application are well understood and agreed upon. Besides, this model can be used for defining test cases of the software application. The communication between the user and the system is the use case diagram represented with an arrow from the actor to the use case.

Screens

Mock-up screens helps the end users better understand how the software application will work.

The functional analysis forms the basis for the software development and project plan.

1.2.2. Phase 2: Technical analysis

The technical analysis or initiation phase consists of the technical architecture and design of the software application, the database design and implementation.

The software architecture describes a set of software elements, the relations between them and the properties of both elements and relations.

An important part of the software architecture are the architectural views, using the 4+1

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architectural view model [5] to describe the software tool.:

> *"4+1 is a view model designed by Philippe Kruchten for "describing the architecture of software-intensive systems, based on the use of multiple, concurrent views". The views are used to describe the system from the viewpoint of different stakeholders, such as end-users, developers and project managers. The four views of the model are logical, development, process and physical view. In addition selected use cases or scenarios are utilized to illustrate the architecture serving as the 'plus one' view. Hence the model contains 4+1 views."*

These views describe the software product from different viewpoints: one for each type of stakeholder.

- ✓ The logical view is concerned with the functionality that the system provides to end-users.
- ✓ The development view illustrates a system from a programmer's perspective and is concerned with software management. It describes the system's components and their interfaces.
- ✓ The process view deals with the dynamic aspects of the system, explains the system processes and how they communicate, and focuses on the runtime behavior of the system. This view also contains the scientific processes developed by the researcher.
- ✓ The deployment view depicts the system from a system engineer's point-of-view. It is concerned with the topology of software components on the physical layer, as well as the physical connections between these components.
- ✓ The description of an architecture is illustrated using a small set of use cases, or scenarios. The scenarios describe sequences of interactions between objects, and between processes. This view is important for system testers.

Another part of the software architecture is the data model design. By means of an UML class diagram we described the entities, the relations between entities, and their attributes as resp. classes, associations, and class fields.

1.2.3. Phase 3-5: Implementation cycle 1, 2, 3

Every implementation cycle describes the development and the implementation of the functionalities for the planned beta release version. After every beta release version EFSA and the EFSA WG PECs in soil test and validate the released version of PERSAM. The results are documented in validation reports. The identified issues of the validation period should be resolved and this means changes in the development and implementation of the tool.

Figure 7 illustrates the implementation cycle on a graphical way.

[5] Kruchten, Philippe (1995). Architectural Blueprints — The "4+1" View Model of Software Architecture. IEEE Software 12 (6), pp. 42-50.

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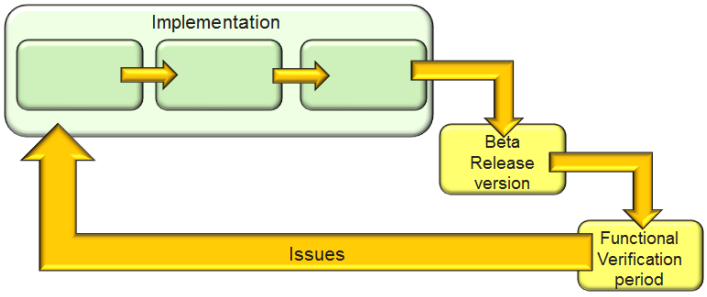

Figure 6: Implementation cycle

1.2.4. Phase 6: Preparation for launch and Delivery-day

During phase 6 we do the preparations for the launch of the final release of the software tool PERSAM. solving the issues of functional verification period 3 finalizing the required documents (user manual, technical report, …).

1.3. Code verification and validation beta releases

1.3.1. Code verification

Code verification during the development is important for the quality assurance of the programmed tool. The code verification will be done on the basis of a number of test cases and by verification of the results comparing the expected output with the actual output *(outcome of other ad-hoc tools).* More information of tests and code verification can be found in the '*Final documented review report'*.

1.3.2. Validation beta releases

The validation of the beta releases is performed in four steps (see Table 2: : defining validation plan, validation phase, feedback phase and acceptance phase. Three beta-versions were released during the project. First beta-version (Tier-1 only) was release in May 2013. Second beta-version was released in August 2013. Thierd beta-version was released in December 2013.

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Table 2: Validation process of beta releases

	Description
Step	
1. Defining validation plan	The validation plan describes a set of use cases for testing the software application and provides a template for the validation reports.
2.Validation phase	EFSA and the EFSA WG PECs in soil test the software application on the basis of the use cases. The test results are documented in the validation reports.
3.Feedback phase	During the feedback phase VITO solves the discovered errors, reported in the validation reports.
4.Acceptance phase	EFSA and the EFSA WG PECs in soil validate the relevant use cases where errors were discovered during the validation process. When the results for this finale validation are positive, EFSA accept the obtained results before starting with the preparations of a new beta release version or the final version of the software application.

Three beta-version were released during the project. First beta-version (TIER-1 only) was released in May 2013. Second beta-version was released in August 2013 and the third beta-version was released in December 2013.

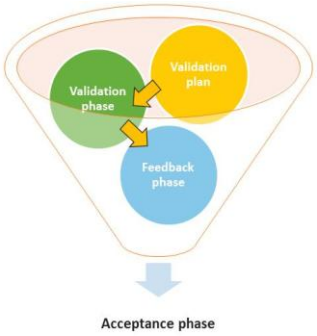

Figure 7: Validation beta releases

1.4. Documentation & implementation of post tool release version control, bug fixing and update

The implementation of a post tool release version control, bug fixing and update includes:

- ✓ Bug fixing & updates for 5 years after the final delivery of the tool
- ✓ Use of source control to track different versions of the software, after the final delivery and acceptance by EFSA of the tool.
- ✓ Release management of software patches or new software versions

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The documentation includes providing solutions for common issues where EFSA desk/ pesticide unit staff is unable to help, e.g. manuals for users having problems with installing or using the tool.

2. IMPLEMENTATION

The implementation is based on the key requirements gathered during the functional analysis. The key requirements consists of functional requirements and non-functional requirements & quality attributes.
More information of the key requirements is available in the appendices: *A. Functional requirements and B. Non-Functional requirements & quality attributes*.

This chapter describes the general architecture, the technology choices, the simple analytical model and the data model. More detailed information is available in the '*Final technical report*'.

2.1. Architecture

The software tool follows a classic 3-tier architecture with the components presentation, business logic, and persistence.

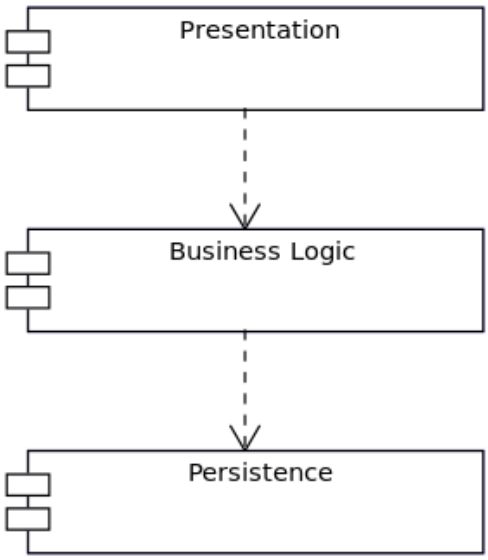

Figure 8 - The 3 layers composing the software tool. Arrows indicate usage: the component where the arrow starts uses functionality offered by the component where the arrow points to.

The persistence component contains all functionality to store, fetch, and update persistent data.

The business logic component implements all business processes of the tool: PEC calculation, input validation, report generation, and data integrity checking.

The presentation component implements the user interface, that is the screens and their components that handle direct user interaction.

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2.2. Technology choices

The tool will be written in Java which allows the development of platform independent software. This will ensure that the developed code will run on all the specified target operating systems with no modification required. Future support for additional operating systems is thereby assured as well.

The following libraries and toolkits are used as well. (Name, URL, version, license, license URL)

Table 3: Used libraries & toolkits

Name	***Version***	***URL***	***License***
Apache Derby	10.10.1.1	http://db.apache.org/derby/	Apache License, Version 2.0
Hibernate	4.1.9	http://www.hibernate.org/	LGPL v2.1
Spring Data JPA	1.3.0	http://projects.spring.io/spring-data-jpa/	Apache License, Version 2.0
JAXB	part of Oracle JVM 1.7.0u25	http://www.oracle.com/us/technologies/java/standard-edition/overview/index.html	Oracle License
Java Swing	part of Oracle JVM 1.7.0u25	http://www.oracle.com/us/technologies/java/standard-edition/overview/index.html	Oracle License
JFreeChart	1.0.16	http://www.jfree.org/jfreechart/	LGPL
jUnit	4.11	http://junit.org/	Eclipse Public License v 1.0
maven	3.0.4	http://maven.apache.org/	Apache License, Version 2.0
iText	2.1.7	http://itextpdf.com/	Apache License, Version 2.0
Nullsoft Scriptable Install System (NSIS)	2.46	http://nsis.sourceforge.net	Common Public License version 1.0
Java Fast Expression Parser	0.1.0	http://jfep.sourceforge.net/	Apache License, Version 2.0

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3. Simple analytical model

All TIER calculations the tool supports, involve – in one way or the other – the application of the simple analytical model (SAM) described in the scientific opinion (EFSA, 2012b).

Each of the actions in this model is the calculation of a simple equation.

The SAM requires a set of input parameters. The value of these parameters is different when it is evaluated for a different endpoint (total soil or liquid phase). For the calculation for the liquid phase endpoint, a number of additional parameters are required. Figure 9 illustrates the input data for the SAM.

The output of the SAM is an array of concentration values. The length of this array is 1 more than the length of the list of t_{avg} values in the input data. The first element of this array is the peak concentration value C_{peak}. The next elements are the C_{TWA} values for each t_{avg} value.

Figure 10 illustrates the steps involved in evaluating the SAM.

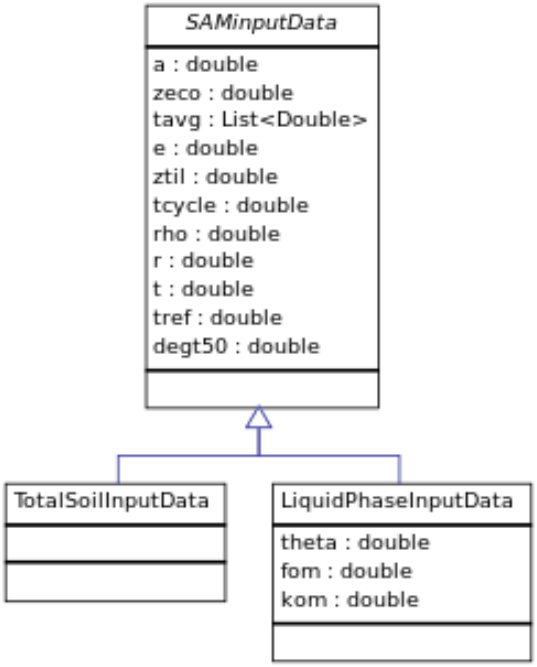

Figure 9 - Input data for the simple analytical model (SAM).

The following table gives an overview of the origin of all the input parameters for the SAM in the different TIERs. The parameters in blue are only required for the liquid phase calculations.

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Table 4: Input parameters for the SAM

Name	Symbol	Unit	TIER 1	Other TIERs
annual application rate	A	kg/ha	user	user
ecotoxicological averaging depth	z_{eco}	dm	fixed list	fixed list
time period since application time over which concentrations are averaged	t_{avg}	days	fixed list	fixed list
dry bulk density	ρ	kg/L	zone specific	spatial data
plough depth	z_{til}	dm	fixed value	fixed value
time between applications	t_{cycle}	days	user selected value from fixed list	user selected value from fixed list
Arrhenius activation energy	E	kJ/mol	substance specific	substance specific
gas constant	R	kJ/mol/K	fixed value	fixed value
Temperature	T	K	zone specific	spatial data
reference temperature	Tref	K	fixed value	fixed value
half life for degradation in soil at 20 ˚C	$DegT_{50}$	days	substance specific	substance specific, possibly function of spatial data
volumetric water content	θ	m^3/m^3	zone specific	spatial data
organic matter content	f_{om}	kg/kg	zone specific	spatial data
organic matter/water distribution	K_{om}	L/kg	substance specific	substance specific, possibly function of spatial data

The provided spatial data does not always have the required unit, in which case it needs to be converted prior to inserting it into the application's database. The following table gives an overview.

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Table 5: Unit conversions

Symbol	Map	Map unit	Target unit	Conversion
ρ	BD_TOP	kg/m^3	kg/L	/ 1000
T_{Arr}	TEFF	˚C	K	+ 273.15
T_{Arit}	TMEAN_YEAR	˚C	K	+ 273.15
θ	THETA_FC_TOP	m^3/m^3	m^3/m^3	
f_{om}	OM_TOP	%	kg/kg	/ 100
	CAPRI_[crop]	%	m^3/m^3	/ 100
	PH_TOP	pH	pH	

The unit of the output parameters is mg/kg for C_T and mg/L for C_L.

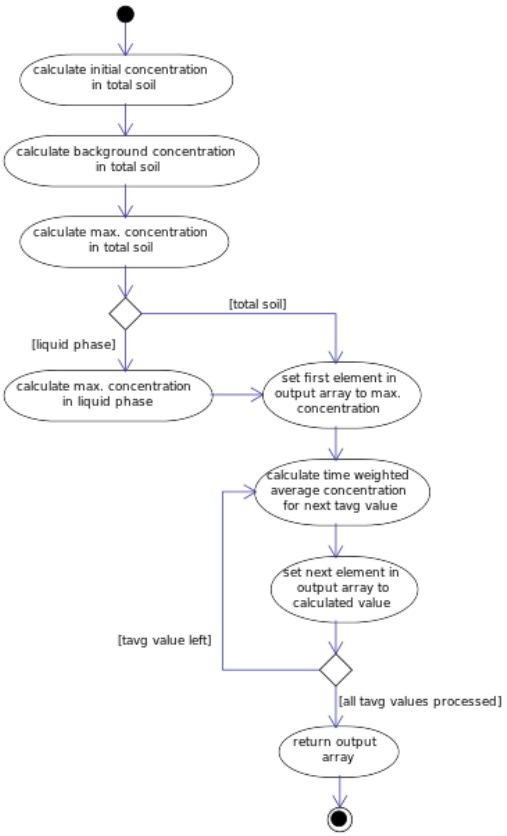

Figure 10 - Steps involved in evaluating the simple analytical model (SAM).

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We now list the equations used in the different steps depicted in Figure 10.

- Calculate initial concentration in total soil:

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

- Calculate background concentration in total soil:

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

where:

$$X = e^{-t_{cycle} f_T k_{ref}}$$
$$f_T = e^{\frac{-E}{R}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)} \ (T > 0\,°C)$$
$$f_T = 0 \ \ (T \leq 0\,°C)$$
$$k_{ref} = \frac{ln2}{DegT_{50}}$$

- Calculate maximum concentration in total soil (= $C_{T,TWA}$ for $t_{avg} = 0$):

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

- Calculate maximum concentration in liquid phase:

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

- Calculate time weighted average concentration:

$$C_{TWA} = \frac{C_{peak}}{t_{avg} f_T k_{ref}} \left(1 - e^{-t_{avg} f_T k_{ref}}\right)$$

where:

$$C_{TWA} = C_{T,TWA} \ \ if \ \ C_{peak} = C_{T,peak}$$
$$C_{TWA} = C_{L,TWA} \ \ if \ \ C_{peak} = C_{L,peak}$$

3.1. Data Model

The data model is depicted on the next page using the UML class diagram.

The data is organized in 2 separate data sources. The white classes represent data inserted and modifiable by the user. The grey classes represent data that is built into the application and needs to be secured against tampering. For the white classes, the application will not communicate with a full-blown database server, but will use a file-based database instead. The (instances of the) grey classes will reside in resource data files.

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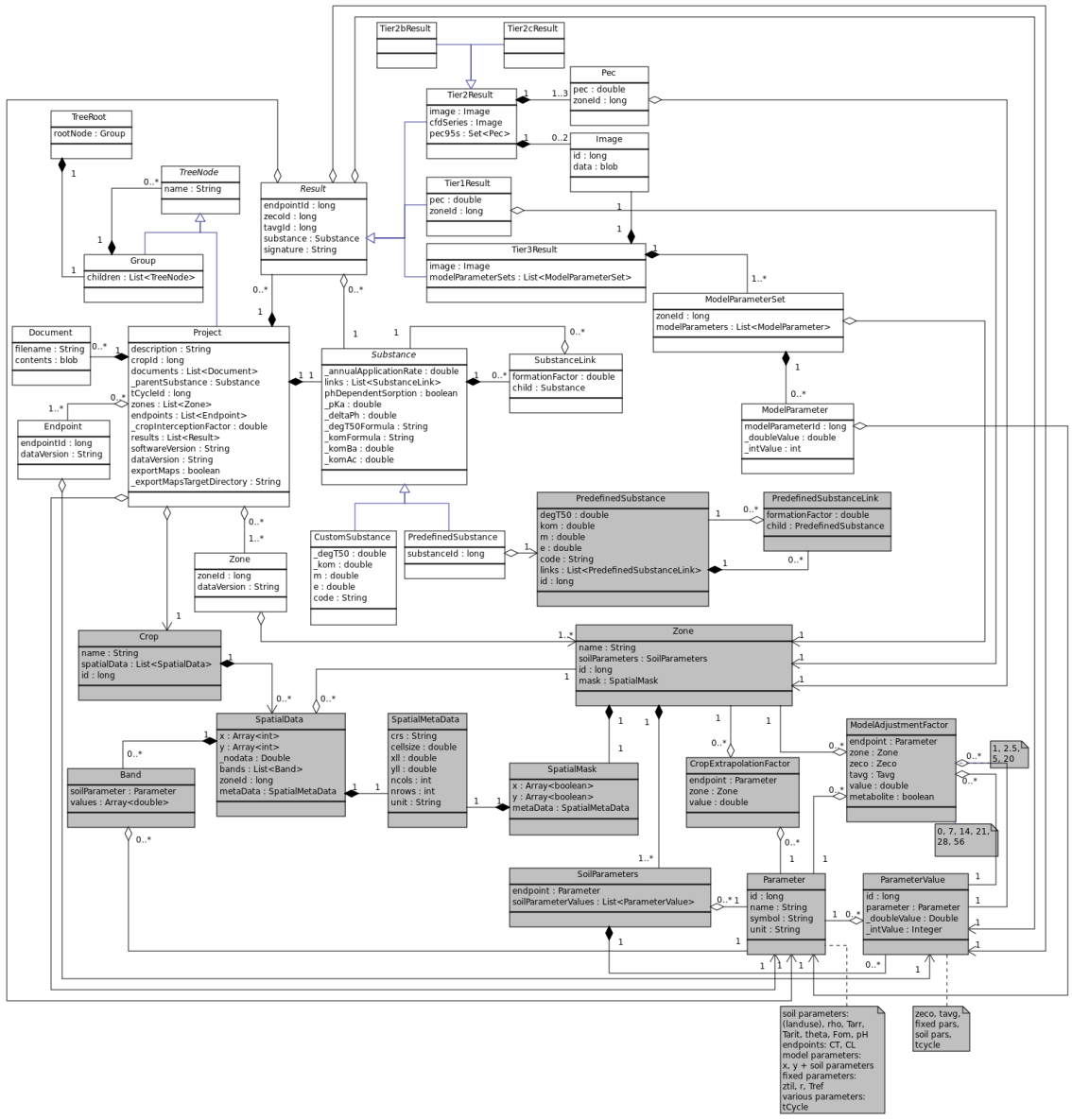

Figure 11 - The data model for the tool. The white classes are used to store the settings made by the user and the calculation results. The grey classes are used to store the built in fixed data.

The associations between the classes need to be interpreted as follows.

- An association flows from the parent class (indicated by a diamond) to the child class (no symbol, or an arrow head). We do not use bi-directional associations.

- Numbers at the endpoints indicate multiplicity: they indicate the number of instances that can exist in an association at each endpoint.

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- A filled diamond indicates a composition: the child's existence depends on the parent's existence: when the parent is deleted, the child must be deleted as well.
    - If the aggregation has no symbol at the child side, the children are fetched along with the parent.
    - If the aggregation has an arrow at the child side, the children are fetched if they are needed (lazy fetching) to avoid unnecessary memory and CPU use.
- An open diamond indicates an aggregation: parent and child can coexist, but if one of them gets deleted, the other one continues to exist. We use 2 kinds of aggregations.
    - Aggregations with no symbol at the child side use a foreign key at the parent to point to the child.
    - Aggregations with an arrow at the child side use a field at the parent which holds an identifier of the child. This can be seen as "an implementation of the foreign key mechanism in the application code". These aggregation types are used when we cannot use foreign keys, because we point to objects that reside in a different database.

If the class name is in *italic*, the class is abstract, that is: a class that cannot be instantiated.

Arrows with triangle shaped heads indicate inheritance.

Parameter names that are prefixed with an underscore (_) can have a null value. The underscore is not a part of the parameter's name. All other parameters must have a value at all time. Lists can be empty.

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4. Project outcome

4.1. Meetings

During the project implementation following meetings have taken place:

Table 6: Overview of the meetings

	Date	Description
Meeting		
Kick-off meeting	13/12/2013	Presentation of the project outline and a first draft version of the functional analysis
Meeting Parma	30/01/2013	Presentation of the functional design of PERSAM and the project plan
Web conference 1	12/03/2013	Presentation of the project status & project progress
Web conference 2	23/04/2013	Presentation of the project status & project progress
Web conference 3	01/07/2013	Presentation of the results of the functional verification period 1 (beta release version 1)
Web conference 4	21/08/2013	Presentation of the project status & project progress and delivery beta release version 2
Web conference 5	01/10/2013	Presentation of the results of the functional verification period 2 (beta release version 2)
Web conference 6	18/11/2013	Determining the most relevant issues for improving the PERSAM software
Web conference 7	12/12/2013	Presentation of the resolved issues and delivery beta release version 3
Web conference 8	26/01/2014	Presentation of the results of functional verification period 3 (beta release version 3)
Web conference 9	25/02/2014	Helpdesk & Hosting PERSAM tool
Web conference 10	08/04/2014	Helpdesk, Hosting PERSAM tool, latest review of the deliverables

4.2. Key issues

Relevant key issues in the project are:

- ✓ The development of the software application corresponding the general objectives.
- ✓ User-friendliness of the software application
- ✓ The performance of the software application

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The final version of PERSAM complies with the key issues

4.3. Identified issues

The identified issues for the period from December 2012 until March 2014 are:

Table 7: Identified issues for period: December 2012 – March 2014

	Issues	Date	Description	Solution	Status
IDS-01	More complicated functionalities for substances	January 2013	The objective is to have a graphical presentation of the substances and metabolites. A second issue was to provide the possibility of defining 4 primary metabolites and 4 secondary metabolites per substance	During the technical analysis we've taken into account the new functionalities and reviewed the project planning.	Resolved
IDS-02	Formula for dealing with pH dependent substances	February 2013	In Tier-2 and higher the possibility to include the pH-dependency of sorption of PPPs is included in the calculations. Providing this as a free-form equation editor to the user is not sufficient and would be a source of error.	The formula for pH dependent sorption using pKa, $K_{om,ba}$, $K_{om,ac}$ and ΔpH (p58 in the Functional Analysis) is built-in into the tool as an option in the Calculation screen (Substances) This functionality will be available in the second beta release.	Resolved
IDS-03	Export generated maps to ESRI ASCII grid files	March 2013	The export of the generated maps requires a lot of disk capacity and therefore it is not advisable to generate automatically the ESRI ASCII files	In the settings tab we provide a checkbox for "export generated maps to ESRI ASCII files". When the user selects the checkbox he should define the destination folder for the generated ESRI ASCII files. The checkbox is by default unchecked.	Resolved

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	Issues	Date	Description	Solution	Status
IDS-04	Divide by zero in analytical model for cases where T_{Arr} is below 0°C	March 2013	In cases where T_{Arr} is below 0°C, there is a division by zero in the analytical model and there are a few cells in the project area with a annual averaged T_{Arr} <0°C	These cells will be filtered out of the input maps for TIER-2B, TIER-2C and TIER-3	Resolved
IDS-05	Project management will be partially available in beta release version 1 and 2.	May 2013	The functionalities: copy project, paste project, import and export project, adding documents to a project are not available yet for the sake of efficient time usage.	These functionalities will be available after the implementation of all tiers otherwise we need to rewrite these functionalities.	Resolved
IDS-06	Beta release version 1does not confirm to the technical requirements of 3.2.1 Installation and running of the technical interim report.	May 2013	Installation of the software tool should not require additional software tools or applications. Beta release version 1 requires the installation of JAVA runtime	Beta release version 2 will provide an installation of the PERSAM tool included the required JAVA runtime files.	Resolved
IDS-07	Unclear how to create a new project	July 2013	When the programme is opened instruction in the tool are missing on how to create a new project. (Ref.VP1-PM-01)	modify settings and results screens, underlying workflow, database layout, export/import functionality, and reporting	Resolved
IDS-08	Reorganize the Settings tab	July 2013	It is not very clear to know which settings are required for which TIERS.(Ref.VP1-ST-01)	relayout settings screen (labeling, positioning of components)	Resolved
IDS-09	No error message for Export generated maps to ESRI ASCII grid file,	July 2013	Export generated maps to ESRI ASCII grid file, doesn't generate an error message (Ref.VP1-ST-02)	This functionality is for the final release and we 'll provide the user of error messages.	Resolved

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	Issues	Date	Description	Solution	Status
IDS-10	Confusing labels In the substance tab	July 2013	Confusing labels: time between applications and annual application rate (Ref.VP1-SUB-01)	Use of tooltips: Tooltip for time between applications: "Period of crop rotation. If a crop is grown for instance every second year, time between applications is 2 years. All applications within one year need to be summed." Tooltip for annual application rate: "The total rate of the substance applied to the crop within one year, without extracting the crop interception."	Resolved
IDS-11	Naming of standard substances 1 – 19 unclear	July 2013	Naming of standard substances 1 – 19 unclear. I would suggest “standard substance 1” and so on or similar.(Ref. VP1-SUB-03)	The naming of the standard substances will be: standard substance 1, standard substance 2	Resolved
IDS-12	Input check on formation factor	July 2013	Add unit for formation factor (which is indeed dimensionless, but should be between 0 and 1) (Ref. VP1-SUB-04)	Providing input check (between 0 and 1)	Resolved
IDS-13	User friendliness of the substance tab	July 2013	Under substances, it could be clearer that you have to click on the squares to fill in the input parameters for the substance. It would help with a note in the model.(Ref.VP1-SUB-05)	add a label 'click to add a substance' in each empty placeholder	Resolved
IDS-14	Using '.' in stead of ','	October 2013	PERSAM: Using '.' in stead of ',' (Ref. VP2-GEN-03)		Resolved

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	Issues	Date	Description	Solution	Status
IDS-15	A threshold value for crop cover of 1% ha/km2	October 2013	If the trigger > 1% then a threshold value for crop cover of 1% ha/km2 should be implemented for calculation and map data (Ref. VP2-GEN-04)		Resolved
IDS-16	The order of results should be always the same	October 2013	The order of results should be always the same (i.e. north, centre, south); now it is sometimes different.(Ref. VP2-GEN-05)		Resolved
IDS-17	Message when creating a group with existing name	October 2013	Creating a new group with an existing name should give a message to the user.(Ref. VP2-GEN-06)	Implement a message	Resolved
IDS-18	pH-dependent sorption doesn't work	October 2013	pH-dependent sorption doesn't work (Ref. VP2-SUB-02)		Resolved
IDS-19	ΔpH may also be negative	October 2013	Define custom calculation; pH dependent sorption: ΔpH may also be negative (Ref. VP2-SUB-05)		Resolved
IDS-20	Formation factor can be more than 1.0	October 2013	Formation factor more than 1.0 needs should be enabled.(Ref. VP2-SUB-06)	Change the input check	Resolved

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	Issues	Date	Description	Solution	Status
IDS-21	Remove CAPRI crop for TIER 1	October 2013	As tier 1 calculation does not account for any crop, all boxes with the CAPRI crop should be removed. (Ref. VP2-TIER1-01)	Remove CAPRI crop	Resolved
IDS-22	Results parameters of TIER-3 are editable	October 2013	In the results detail of TIER-3: Model parameters are editable on double clicking! This should indeed not be the case (Ref. VP2-TIER3-02)		Resolved
IDS-23	PDF- reports: scenario adjustment factors and model adjustment factors, not relevant for all tiers	November 2013	The tables on the scenario adjustment factors and model adjustment factors should not be repeated at all tiers, only where they are actually used (Ref. REP-GEN-01)	Table on the scenario adjustment factor -> only in the report of TIER-1 Table on the model adjustment factors -> only in the reports of TIER-1, TIER-2B and TIER-2C	Resolved
IDS-24	PDF-reports: Remove the units (mg/kg) and (mg/l) in the headers of the table on the scenario adjustment factor.	November 2013	Remove the units (mg/kg) and (mg/l) in the headers of the table on the scenario adjustment factor. These units give the false impression that they apply to the scenario adjustment factor which is dimensionless (Ref. REP-GEN-02)		Resolved
IDS-25	PDF-reports: the values of z_eco are wrong	November 2013	On all the front pages of the reports, the values of z_eco are wrong: zeco: 0.1; 0.2; 0.5; 2 cm (Ref. REP-GEN-03)		Resolved

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	Issues	Date	Description	Solution	Status
IDS-26	PDF-reports & Replace the label Effect of crop interception (incl.wash-off) door Fraction that reached the soil	November 2013	Replace the label Effect of crop interception (incl.wash-off) door Fraction that reached the soil(Ref. REP-GEN-04)	Change the label in the reports and in the PERSAM software	Resolved
IDS-27	TIER-3 results detail: add pH and crop cover	November 2013	In the results detail of TIER-3: Model parameters: pH and crop cover (ha/km2) of the selected scenario should be given as well (Ref. VP2-TIER3-01)	Add pH and crop cover to the results detail window of TIER-3	Resolved
IDS-28	Installation: user can select a personal profile folder.	November 2013	PERSAM installation: providing the opportunity that the user can select a personal profile folder.(Ref. VP2-GEN-01)		Resolved
IDS-29	Substances: Only fraction of organic matter and pH are relevant in the calculation window	November 2013	In the custom calculation window remove all the spatial parameters, except fraction of organic matter (om) [kg/kg] and pH [-] (Ref. VP2-SUB-04)		Resolved
IDS-30	F soil, max cannot be higher than 1	January 2014	Input validation for F soil, max between 0 and 1		Resolved
IDS-31	The results tab of TIER-2C : wrong results	January 2014	The results tab of TIER-2C presents not the right results conform the output files		Resolved

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	Issues	Date	Description	Solution	Status
IDS-32	Export issues	January 2014	- Present the results in the same units as on the screen (ex. on the screen in cm)- Add the units to the labels		Resolved
IDS-33	Only include cells with dominant land use	January 2014	Only include cells with dominant land use = annual crops		Resolved
IDS-34	when exporting PDFs or CSVs: remember path and start in that path next time	January 2014	When exporting PDFs or CSVs: remember path and start in that path next time		Resolved

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RESULTS

1. 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.

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

Figure 12: Project management tree

1.1. Group

A group is a collection of one or more projects in the tree structure.
Group operations include create a new group, modify an existing group (rename) and delete a group.

Figure 13: Create a new group

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1.2. Project

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

When clicking on a project in the project tree manager at the left side of the screen, the project main screen appears. In this screen, the user can modify the project's name, its description, and the documents attached to the project. At the bottom right of the screen, there are 2 buttons that are disabled if no changes have been made. As soon as a change has been made, the buttons become active. Clicking the undo button will revert all changes made. Clicking the save button will persist the changes.
In the project tree, a fixed set of sub-items of the project are shown: fixed parameters, settings, substances, TIER-1, TIER-2B, TIER-2C and TIER-3.

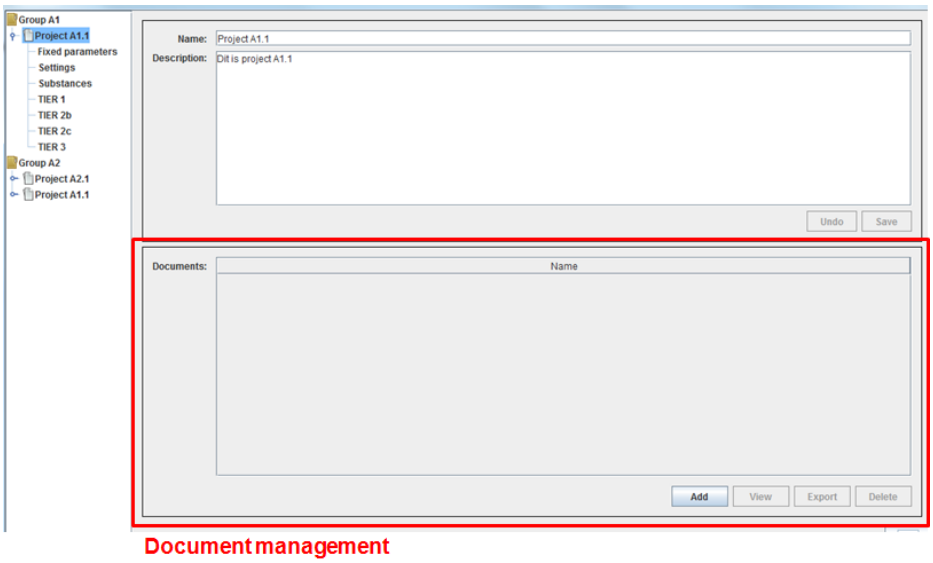

Figure 14: Project main screen

In the project main screen 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 15 shows how the user can add a document to a project. The user clicks on the 'Add' button and a popup window appears where the user selects a particular document. Then he clicks on 'Open' and the document is added to the project.

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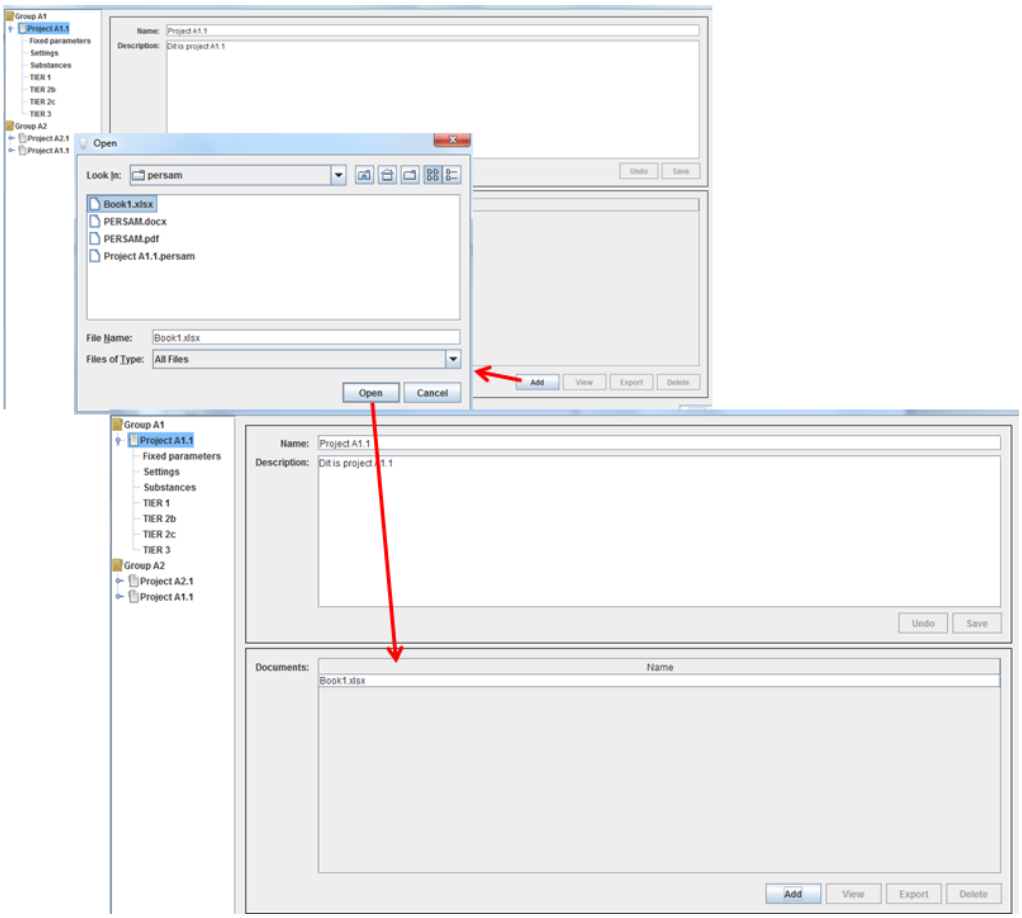

Figure 15: Add a document

Thereafter the user can view the document by selecting a document and clicking on the 'View' button.

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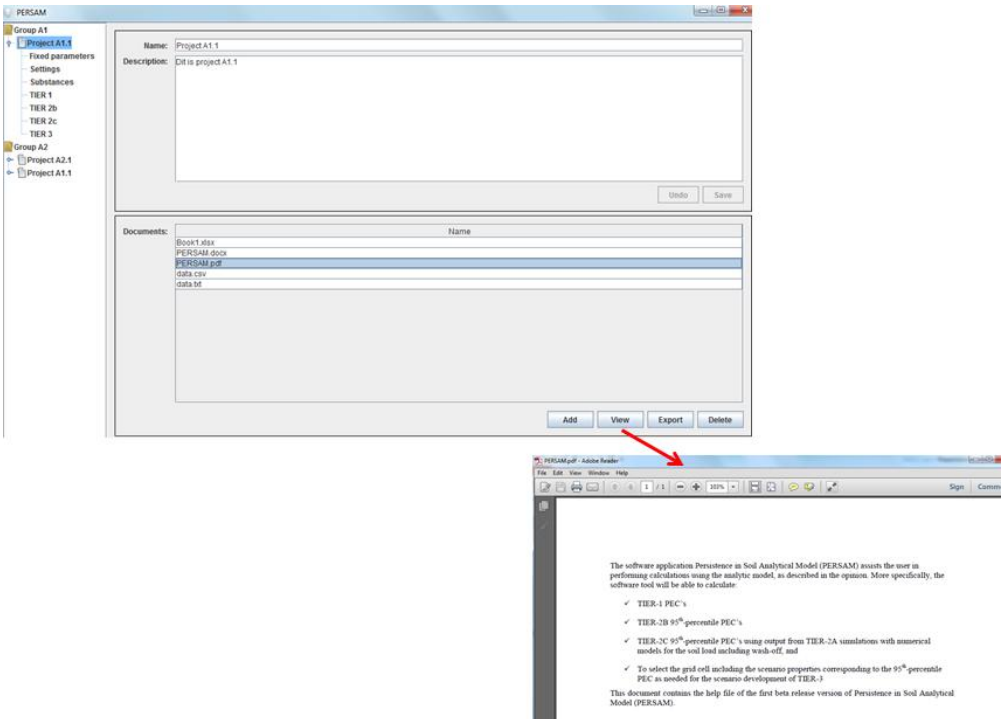

Figure 16: View a PDF file

Project operations are defining a new project, open an existing project, modify and save a project, copy and paste a project, delete a project, import and export a project.

Figure 17 show how the user can copy and paste a project. The user selects an existing project, right click and he selects 'Copy project'. The application makes a copy of the project to clipboard.

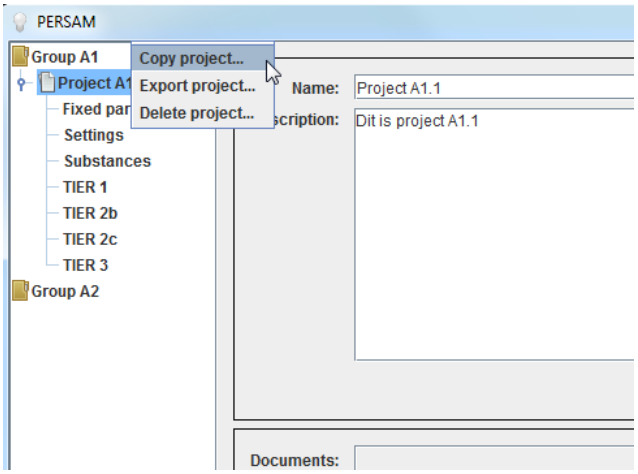

Figure 17: Project management - Copy project

Thereafter the user selects the group where he wants to place the copied project, right click and he

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selects 'Paste project'. The copied project is placed in the group and the user can rename the project.

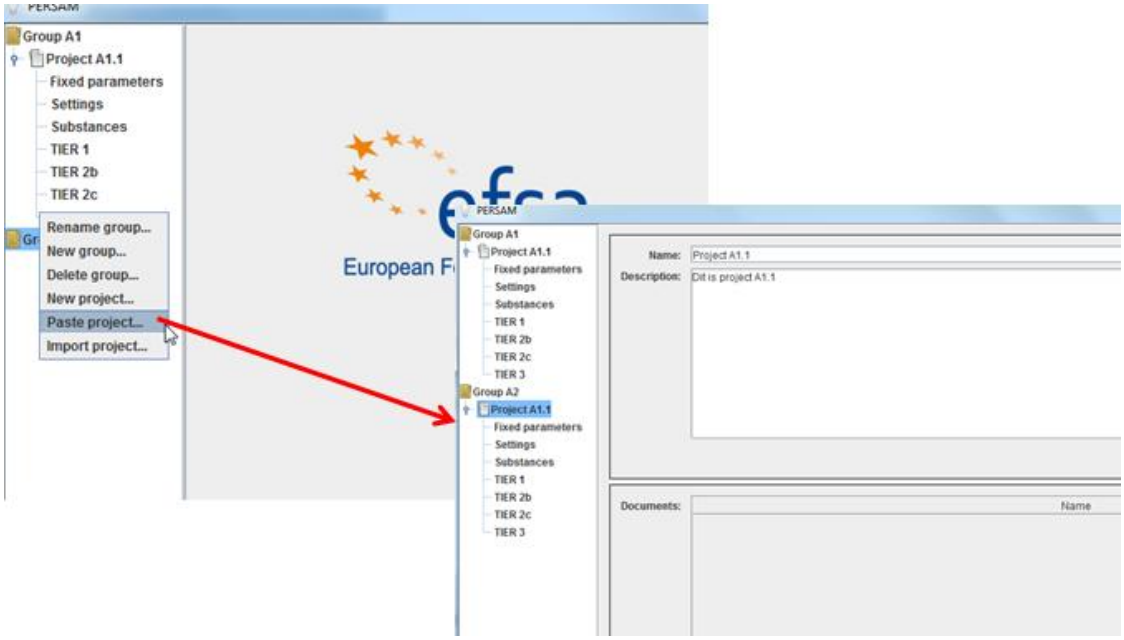

Figure 18: Project management - Paste project

2. Fixed parameters

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

Table 8: Fixed parameters

	Symbol	Unit	Default values
Parameter			
Ecotoxicological averaging depth	z_{eco}	cm	1; 2.5; 5; 20
Plough depth	z_{til}	cm	20
Gas constant	R	$kJ.mol^{-1}.K^{-1}$	0.008314
Reference temperature	T_{ref}	K	293
Time period since application over which concentrations are averaged	t_{avg}	days	0; 7; 14; 21; 28; 56

Figure 19 shows a screenshot of the fixed parameters.

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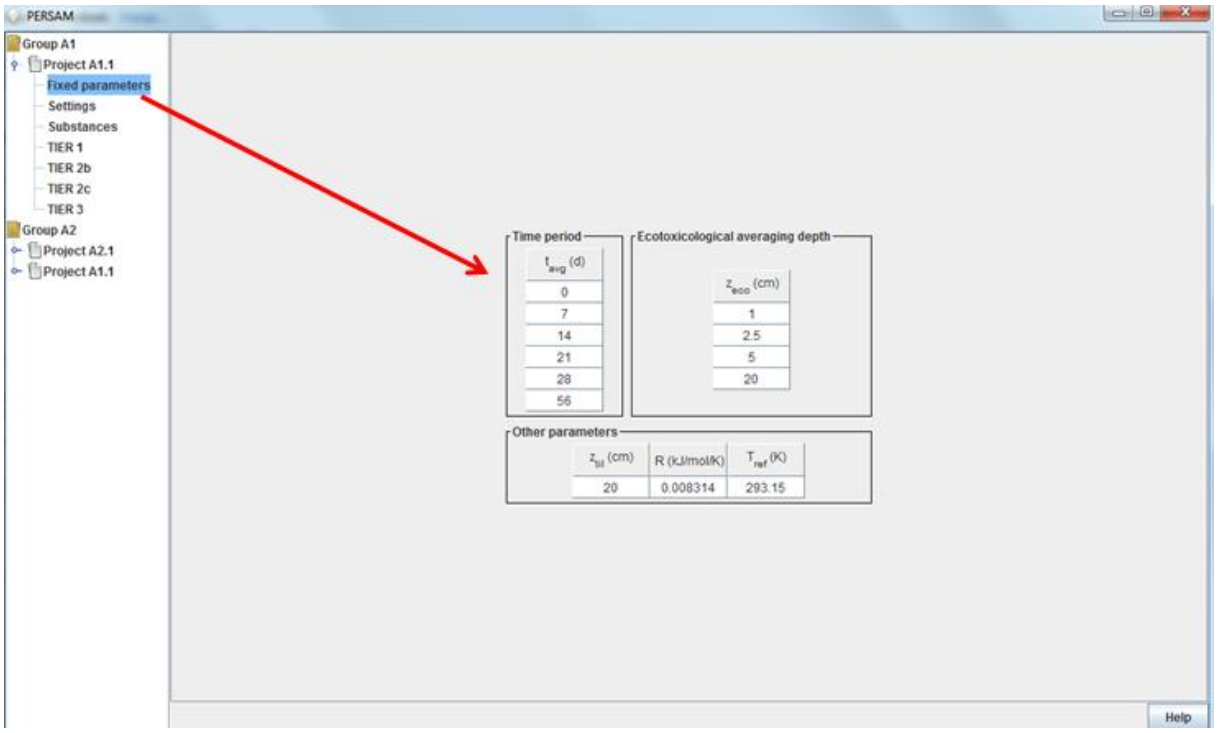

Figure 19: Fixed parameters

3. Settings

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

- The calculation can be done for several zones. At least 1 zone must be selected.
- Several endpoints can be calculated. At least 1 endpoint must be selected.
- The CAPRI crop for which the calculations must be done.
- For TIER 2c, the user must enter the formation factor that reaches the soil to use here. This parameter is not used in the other TIERs.

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

Following table gives an overview of the selection parameters.

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Table 9: Selection parameters

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

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

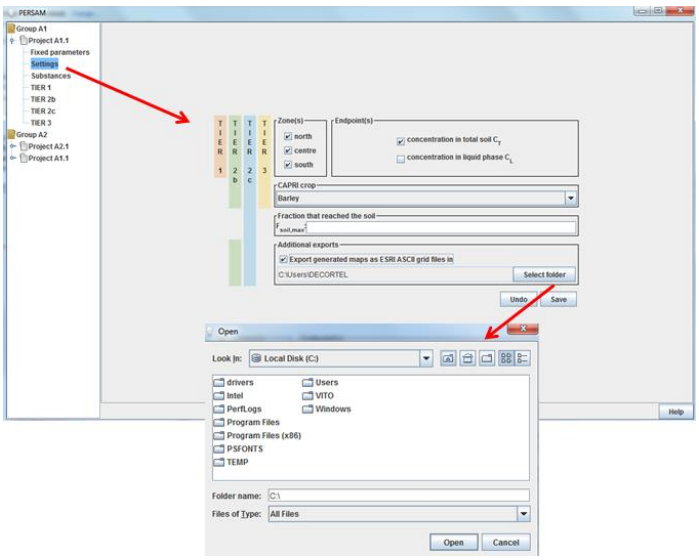

Figure 20: Settings section

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4. Substances

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

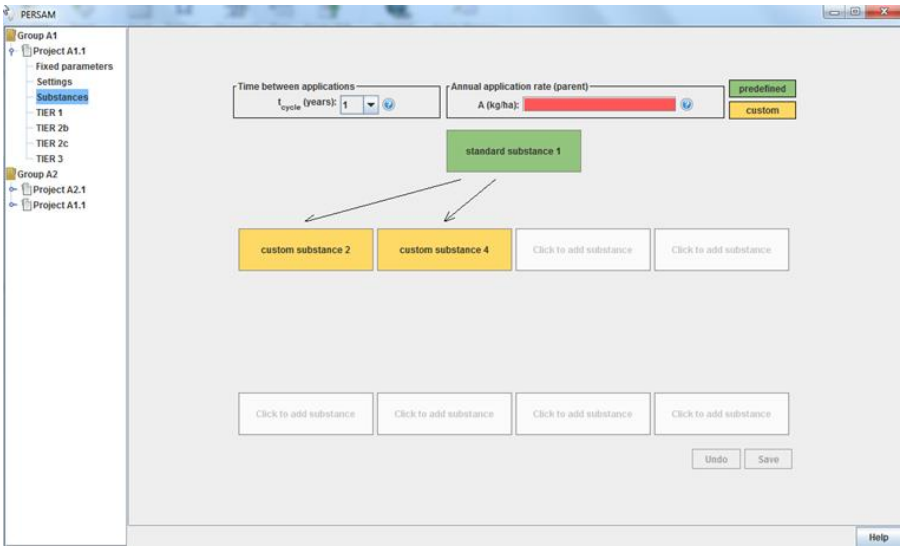

Figure 21: Substances section

A substance (parent or metabolite) is configured by clicking on a place holder in the tree. The tool contains a number of predefined substances with a fixed configuration. Apart from these, the user can also define custom substances. The color of the place holders indicates which of those 2 types of substances is used (green: predefined substance, orange: custom substance).
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 10: Substance-specific parameters

	Symbol	Unit	Default value
Parameter			
Half life for degradation of the substance	DegT50	days	
Organic matter/water distribution coefficient	K_{om}	l/kg	
Organic carbon/water distribution coefficient	K_{oc}	l/kg	

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Molar mass	M	$g.mol^{-1}$	
Arrhenius activation energy	E	$kJ.mol^{-1}$	65.4
Formation fraction metabolite	F_f		
Annual application rate	A	kg/ha	

The user can configure a predefined or a custom substance, delete a substance, configure links between substances and delete links between substances.

Figure 22 shows how the user defines a parent substance. The user clicks on a place holder in the tree and the screen 'Configure substance' appears. Then the user selects one of the build in substances in the drop down list and the screen shows automatically the related parameters of the selected substance. Thereafter he clicks on 'OK' and the parent substance is visible in the tree structure.

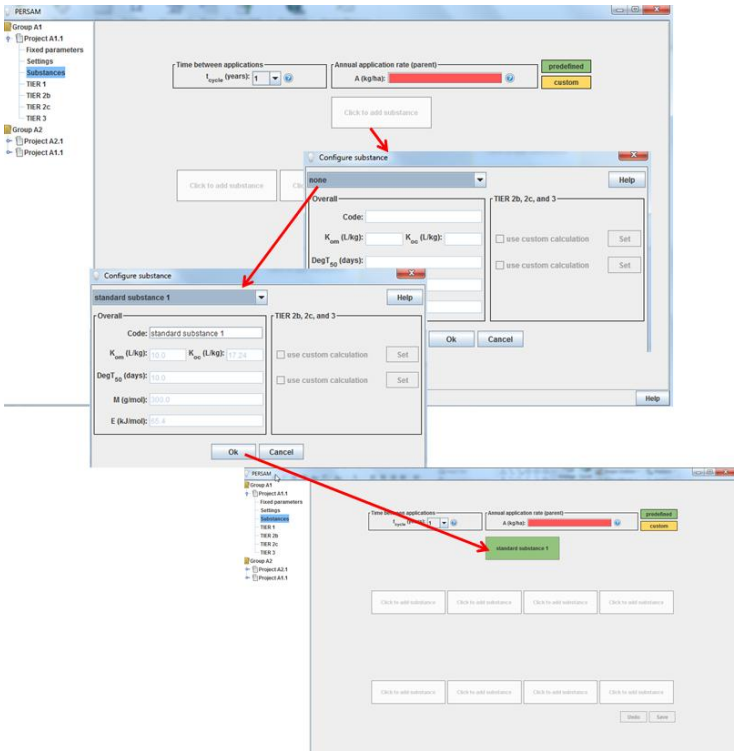

Figure 22: Define the parent substance

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Next step is defining a metabolite. The user selects again a place holder and selects one of the build in substances in de window ‘Configure substance’. The screen shows automatically the related parameters, the user changes one of this parameters, defines a new code that identifies the substance and clicks finally on ‘OK’. The user has defined a customized metabolite.

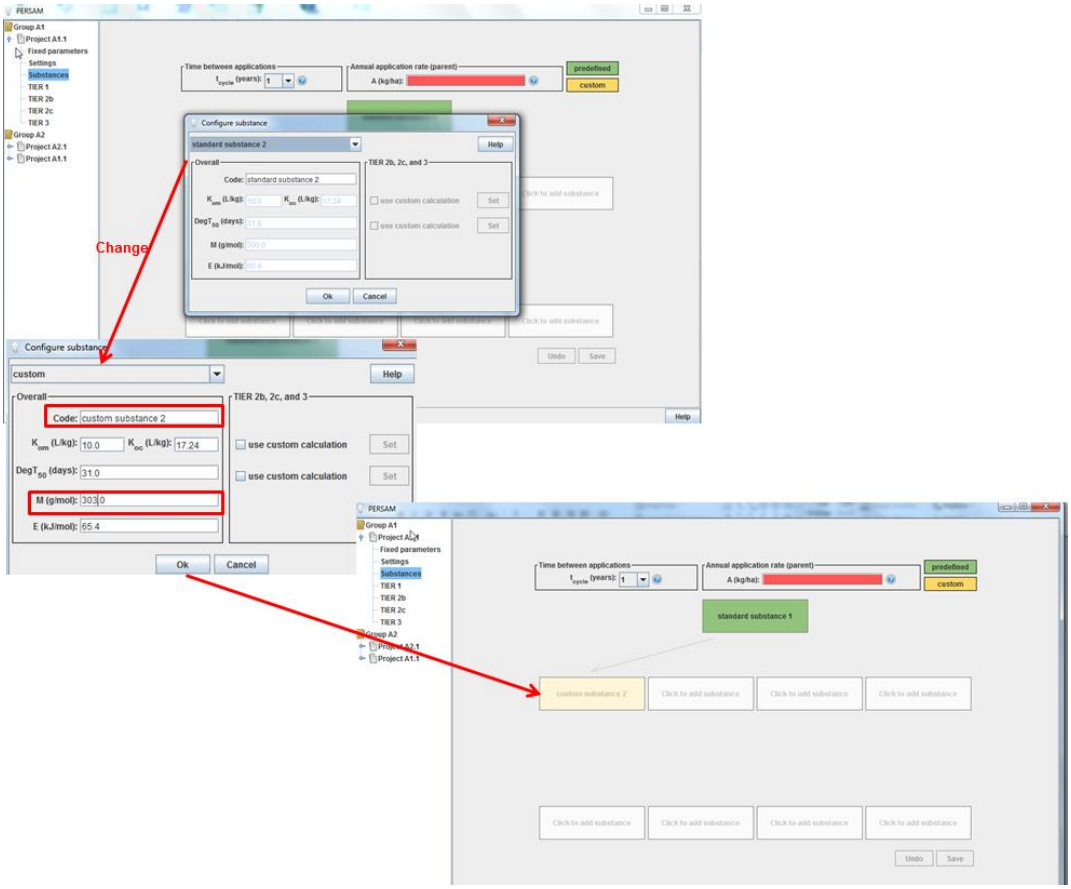

Figure 23: Configure a customized metabolite, starting from a predefined substance

Finally the user configures the link between the parent substance and the metabolite by clicking on an arrow between the two place holders. The dialog window ‘Configure link’ appears. The source and target substance fields are informative and cannot be changed. The user enables the checkbox ‘Link enabled’, defines a formation factor and clicks on ‘OK’.

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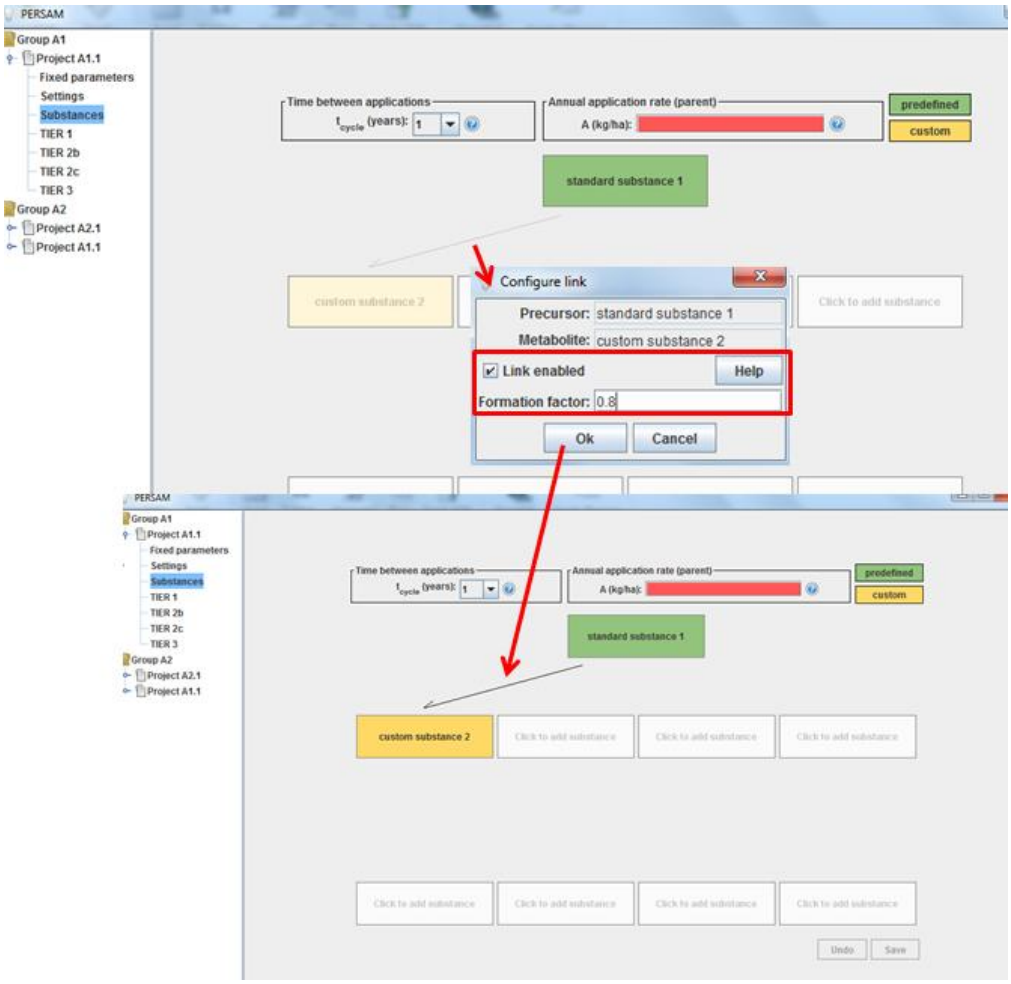

Figure 24: Configure a link

In the 'Configure substance' window the user has the posibility to define relationships between Kom, DegT50 and soil properties. The user selects the checkbox 'Use custom calculation' for Kom or for DegT50 and then clicks on the related set button. In the window 'Define custom calculation' the user can define a custom calculation based on a spatial parameter or use the pH dependent sorption.
The formula for pH dependent sorption is:

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

pKa: negative logarithm of the dissociation constant
ΔpH: pH correction factor

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

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

Table 11: Spatial parameters available in the 'Define custom calculation' window

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

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

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

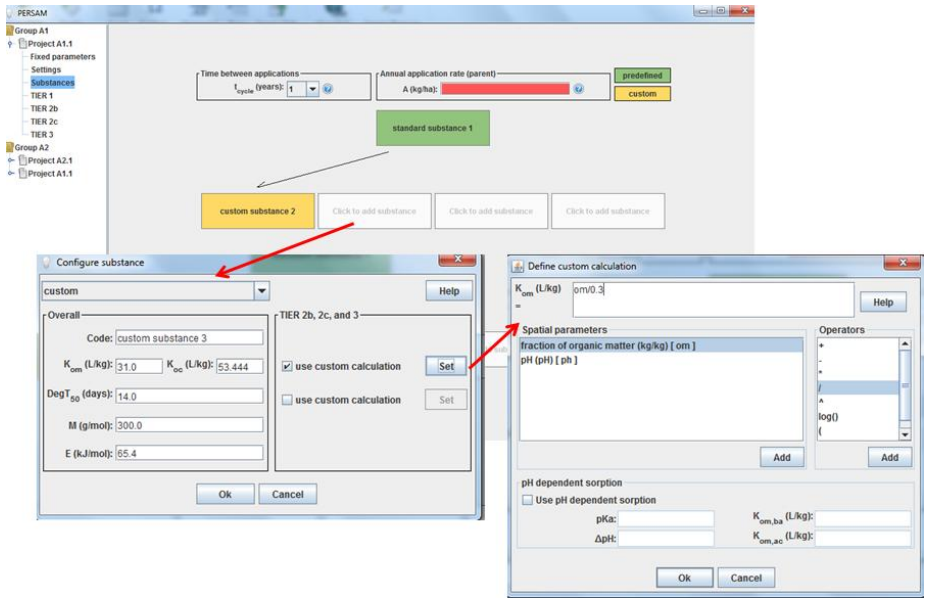

Figure 25: Define custom calculation for Kom

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5. TIER-1

5.1. Overview tab

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

The TIER-1 section is shown in following figure.

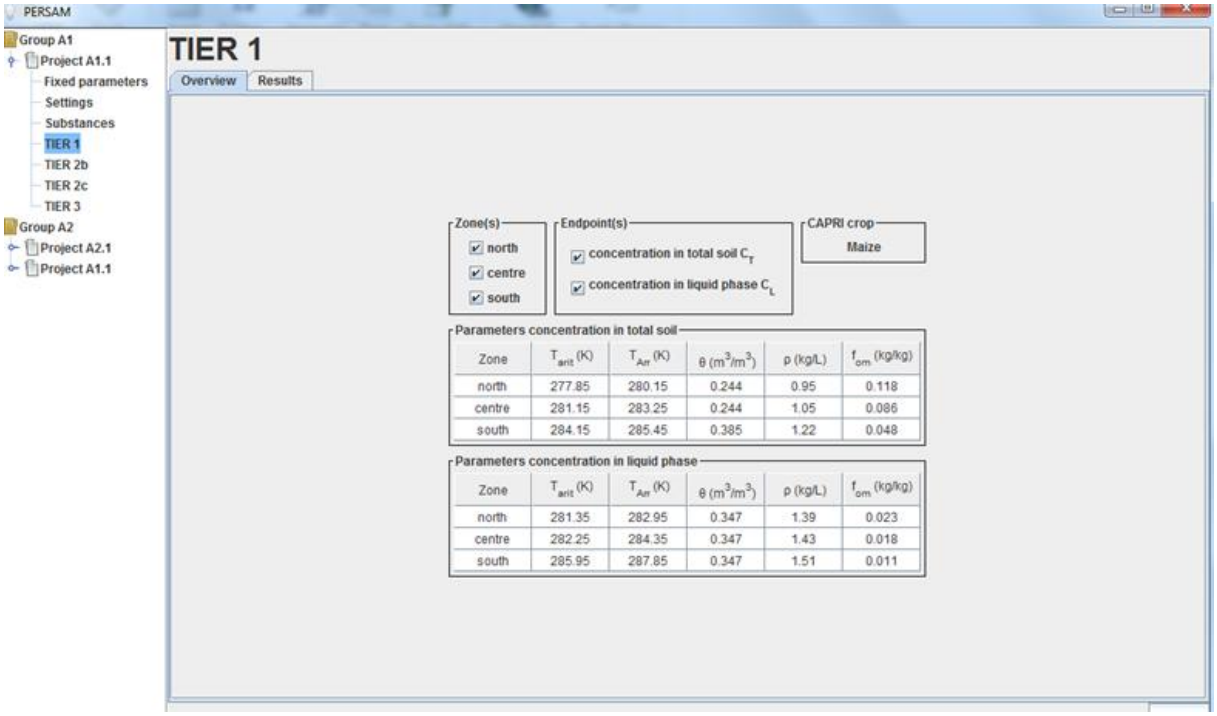

Figure 26: TIER-1 – overview tab

This screen consists of 2 tabs: overview and results. The overview tab (see Figure 26) shows the configured settings and the zone and endpoint dependent parameter values that will be used in the calculations.

Table 12: presents the zone and endpoint dependent parameters.

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Table 12: Parameters dependent on the zone and endpoint

	Symbol	Unit
Parameter		
Temperature T_{Arit}	T_{Arit}	°C
Temperature T_{Arr}	T_{Arr}	°C
Volumetric water content	θ	$m^3\ m^{-3}$
Dry bulk density	ρ	$Kg\ L^{-1}$
Organic matter content	f_{om}	kg/kg

5.2. Results tab

The results tab shows the calculated results for TIER-1 corresponding to the selected parameters and substances.

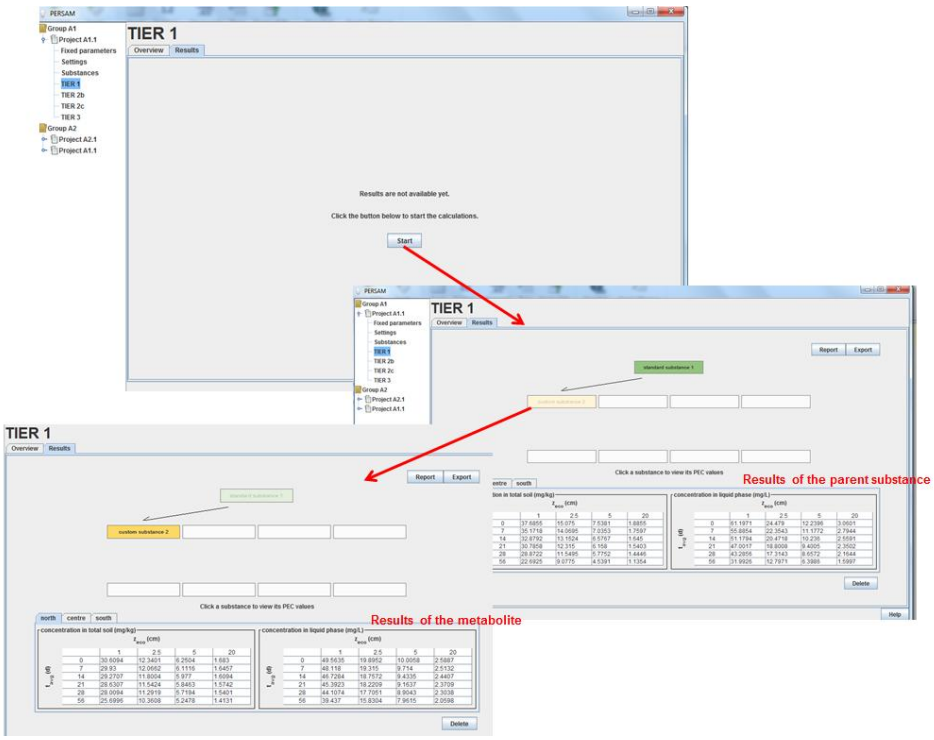

Figure 27: Performing TIER-1 calculations & Results tab

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5.3. TIER-1 calculations

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

5.3.1. Calculations

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

Step 1: calculation of the initial concentration in total soil

Formula 1

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

With:

Table 13: Parameters of formula $C_{T,ini}$

	Symbol	Unit	Default values/Input
Parameter			
Initial total concentration in soil	$C_{T,ini}$	$mg.kg^{-1}$	Formule [1]
Ecotoxicological averaging depth	z_{eco}	cm	1; 2,5; 5; 20
Annual application rate	A	$kg.ha^{-1}$	Input field tab Substances
Dry bulk density	ρ	$kg.L^{-1}$	Soil-specific parameter – tab TIER-1 (*more info see Appendix E*)

Step 2: background concentration in soil just before next application

Formula 2:

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

Formula 3:

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

Formula 4:

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

$$T < 0°C \quad f_T = 0$$

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Formula 5:

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

With:

Table 14: Parameters used in step 2

	Symbol	Unit	Default values/Input
Parameter			
Background concentration in soil just before next application	$C_{T,plateau}$	$mg.kg^{-1}$	Formula 2
Ecotoxicological averaging depth	z_{eco}	cm	1; 2,5; 5; 20
Plough depth	z_{til}	cm	20
Initial total concentration in soil	$C_{T,ini}$	$mg.kg^{-1}$	Step 1
fraction of the dose left at the moment of the next application	X		Formula 3
Time between applications	t_{cycle}	days	365; 730; 1095
Correction factor for temperature	f_T		Formula 4
degradation rate coefficient at reference temperature	k_{ref}	$days^{-1}$	Formula 5
Arrhenius activation energy	E	$kJ.mol^{-1}$	Default 65,4; input field in Substances
Gas constant	R	$kJ.mol^{-1}.K^{-1}$	0,008314
Reference temperature	Tref	K	293
Arrhenius weighted average soil temperature	T_{Arr}	K	Corresponding to parameter T in formula 4 Soil-specific parameter (*more info see Appendix E*)
Half life for degradation in soil at 20°C	DegT50	days	Substance-specific parameter

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Step 3: calculation of the maximum concentration in soil

Formula 6:

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

With:

Table 15: Parameters in formula $C_{T,peak}$

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

Step 4: calculation of the maximum concentration in liquid phase

Formula 7:

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

With:

Table 16: Parameters in formula $C_{L,peak}$

	Symbol	Unit	Default values/Input
Parameter			
Maximum total concentration in soil	$C_{T,peak}$	$mg.kg^{-1}$	Formula 3
Volumetric water content	θ	$m^3.m^{-3}$	Soil-specific parameter –(*more info see Appendix E*)
Dry bulk density	ρ	$kg.L^{-1}$	Soil-specific parameter (*more info see Appendix E*)
Organic matter content	f_{om}	$kg.kg^{-1}$	Soil-specific parameter (*more info see Appendix E*)
Organic matter/water distribution coefficient	K_{om}	$L.kg^{-1}$	Substance-specific parameter
Maximum liquid concentration in soil	$C_{L,peak}$	$mg.L^{-1}$	Formula 7

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Step 5: calculation of the TWA concentration in total soil

Formula 10:

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

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

Table 17: Parameters in formula $C_{T,TWA}$

	Symbol	Unit	Default values/Input
Parameter			
Time weighted average (TWA) total concentration in soil	$C_{T,TWA}$	$mg.kg^{-1}$	Formula 10
Maximum total concentration in soil	$C_{T,peak}$	$mg.kg^{-1}$	Step 3
Time period since application time over which concentrations are averaged	t_{avg}	days	7; 14; 21; 28; 56 days
Correction factor for temperature	f_T		Formula 4
Degradation rate coefficient at reference temperature	k_{ref}	$days^{-1}$	Step 2
Maximum liquid concentration in soil	$C_{L,peak}$	$mg.L^{-1}$	Step 5
Time weighted average (TWA) liquid concentration in soil	$C_{L,TWA}$	$mg.L^{-1}$	Formula 10

Step 6: calculation for metabolites

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

Formula 13:

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

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Formula 14:

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

With:

Table 18: Parameters in formula $A_{met,1}$ and $A_{met,2}$

	Symbol	Unit	Default values/Input
Parameter			
Formation fraction for the first metabolite	$F_{f,1_p}$		Substance-specific parameter
Formation fraction for the second metabolite	$F_{f,2_p}$		Substance-specific parameter
Molar mass of the first metabolite	$M_{met,1}$	$g.mol^{-1}$	Substance-specific parameter
Molar mass of the second metabolite	$M_{met,2}$	$g.mol^{-1}$	Substance-specific parameter
Molar mass of the parent substance	M_{parent}	$g.mol^{-1}$	Substance-specific parameter
Equivalent annual application rate first metabolite	$A_{met,1}$	$kg.ha^{-1}$	Formula 13
Annual application rate	A	$kg.ha^{-1}$	Input field tab Substances
Equivalent annual application rate second metabolite	$A_{met,2}$	$kg.ha^{-1}$	Formula 14

5.3.2. Applying scenario adjustment factor and model adjustment factor

5.3.2.1. Scenario adjustment factors

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

The opinion (EFSA, 2012b) advises to use the maximum values for each endpoint and regulatory zones (third and fifth column in table 13 and table 14). The extrapolation factors should be applied in step 3, step 4 and step 5 of the calculation.

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Table 19: Scenario adjustment factors for CAPRI crops

	$C_{T,peak}$ [(a)]	$C_{L,peak}$ [(a)]
Zone		
North	3.0	2.0
Centre	2.0	1.5
South	2.0	1.5

(a) rounded up at 0.5 steps

5.3.2.2. Model adjustment factors

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

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

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

These are used for the parent substances and the metabolites. Later on a separate set of model adjustment factors may be provided to the metabolites if this is justified scientifically.

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

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

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

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

6. TIER-2B

6.1. Overview tab

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

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

Before starting the calculations of TIER-2B, the user selects a Capri crop in the settings tab and defines in the substance tab a substance with the related metabolite(s) and the annual application rate.

The overview tab of TIER-2B is shown in following figure.

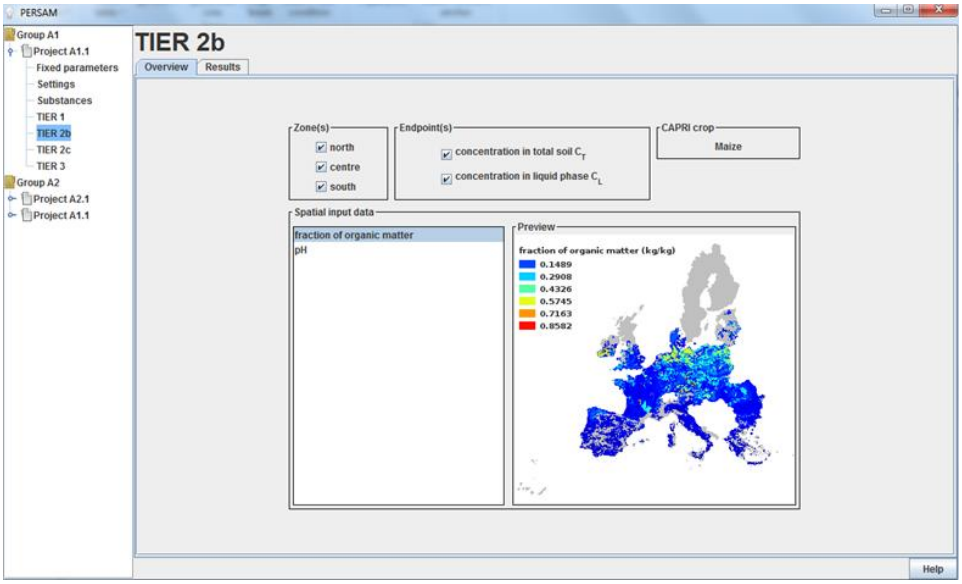

Figure 28: TIER-2B - overview tab

The overview tab presents the selected zone(s), endpoint(s) and Capri crop and these fields are disabled. In a second part of the overview tab the user has the possibility to preview the spatial input data by selecting one of these maps.

6.2. Results tab

The user starts the calculations and the results tab shows the calculated results for TIER-2B corresponding to the selected parameters and substances (see Figure 29: Performing TIER-2B calculations & results tab). The table contains a field for each combination of endpoint, ecotoxicological averaging depth and time window. The user can view extended results of a particular combination by clicking on the cell and then a detail window appears containing the 95th spatial percentile of calculated PECs for the regulatory selected zone with the related cumulative distribution graph and map.

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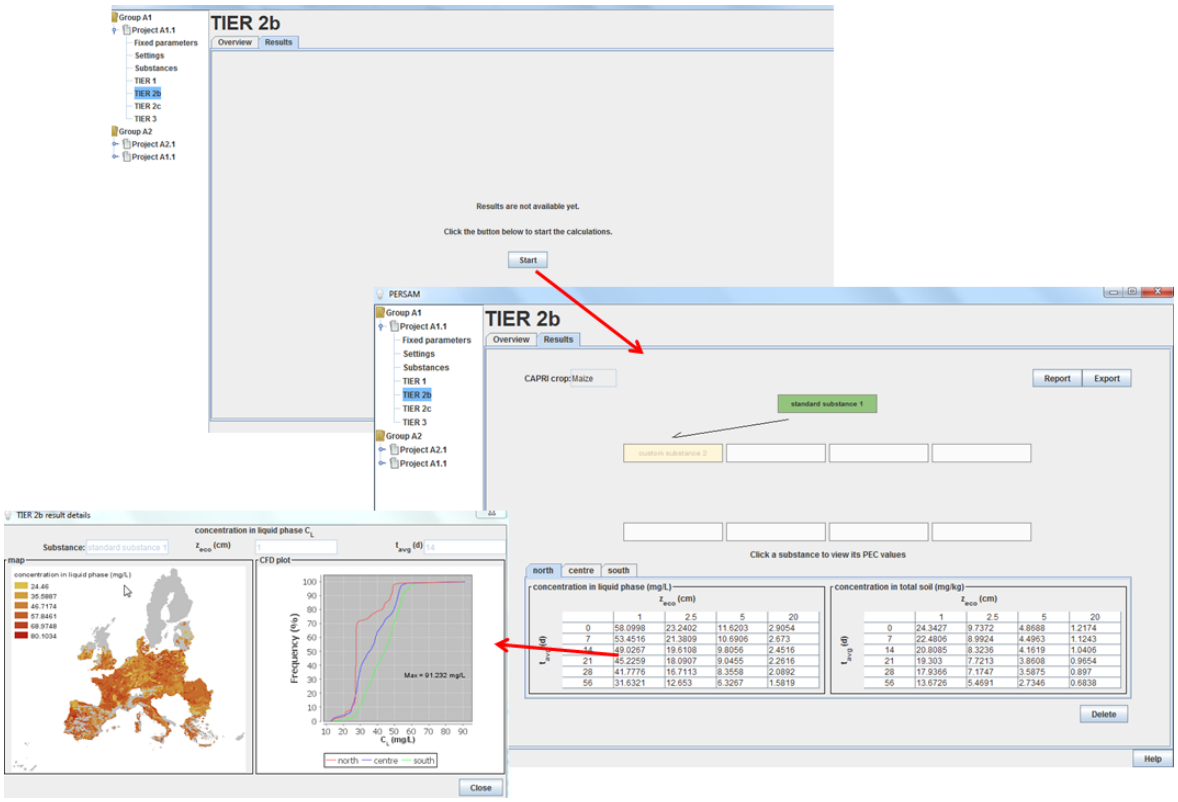

Figure 29: Performing TIER-2B calculations & results tab

6.3. TIER-2B calculations

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

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

7. TIER-2C

TIER-2C is almost analogue to TIER-2B, only that the user should define an extra parameter $F_{soil\ ,max}$ which must be retrieved from model calculations outside of this tool or alternatively through look-up tables to be developed by the EFSA WG on PECs in soil.

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

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

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

The user defines $F_{soil,max}$ in the settings tab.

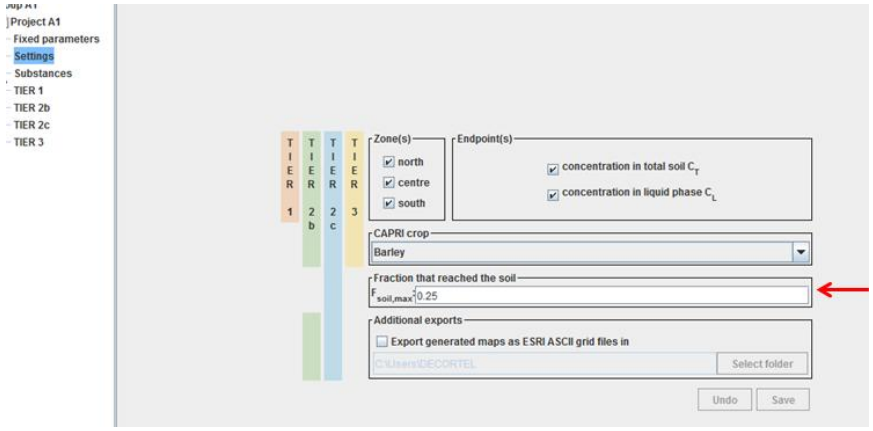

Figure 30: Settings tab – Formation factor that reached the soil

The formation factor that reaches the soil is also provided on the overview tab.

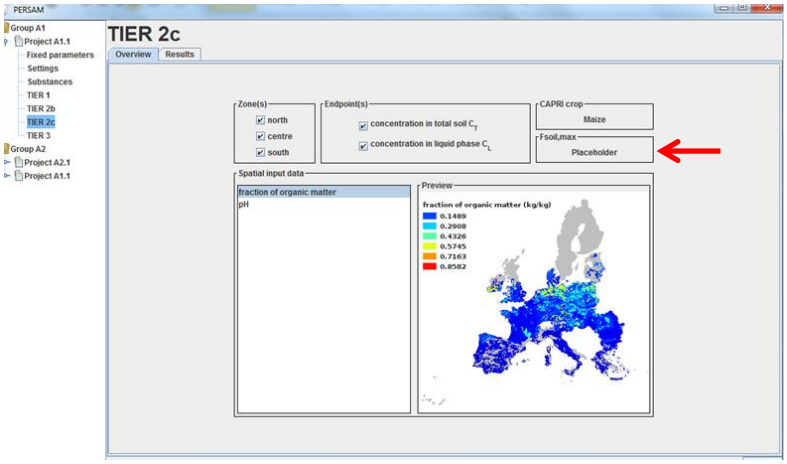

Figure 31: TIER-2C - overview tab

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8. TIER-3

8.1. Overview tab

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

TIER-3 contains an overview and a results tab. The overview tab is analogue to TIER-2B.

8.2. Results tab

The results tab of TIER-3 contains a table with the green cells which indicates whether there results are available (see Figure 32: TIER-3 - results tab). The user can view the result of a particular cell (a combination of ecotoxicological averaging depth, time window and endpoint) by clicking on the cell and there will appear a result window containing the model parameters for the TIER-3 scenario and the vulnerability map showing the calculated vulnerability indices and the location of the grid cell corresponding to a 95% vulnerability.

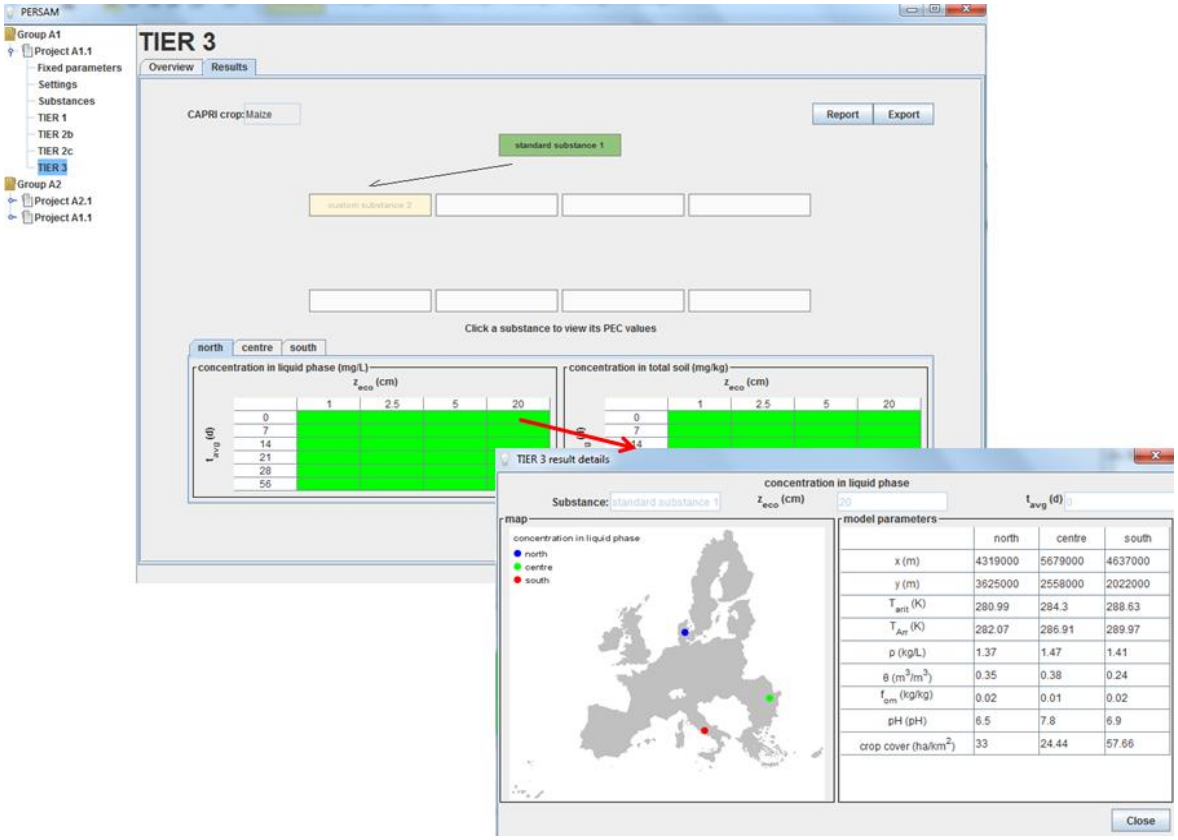

Figure 32: TIER-3 - results tab

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8.3. TIER-3 calculations

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

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

- ✓ Apply the land-use mask of the annual crops to all maps.
- ✓ Based on the map of the relevant crop or crop group, create individual maps for each endpoint (e.g. *CL,peak* or *CT, peak* or any of the TWA concentrations for *zeco* of 1, 2.5, 5 or 20 cm) and for the *DegT50 - Kom* properties of this substance; so this gives only one map that applies only to the type of concentration considered in one of the regulatory zones.
- ✓ Transform the concentration map into a vulnerability map by assigning to each grid cell the percentile corresponding to its concentration. In the calculation of this percentile, each 1×1 km2 pixel should get a weight that is proportional to the fraction of surface area grown with this crop or crop group.
- ✓ Select from the vulnerability map the grid cell with the percentile that is closest to 95%.
- ✓ Use this grid cell to parameterize the scenario.

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9. Reporting & export results

PERSAM generates PDF reports of the results of TIER-1, TIER-2B, TIER-2C and TIER-3 and provides the functionality to export the results to a CSV file. These functionalities are provided on the results tab of every TIER.

Figure 33 shows the generation of a PDF report for TIER-1. The information of the PDF reports can be used in other WORD documents, by selecting the text in the PDF report and copy/paste to the word document.

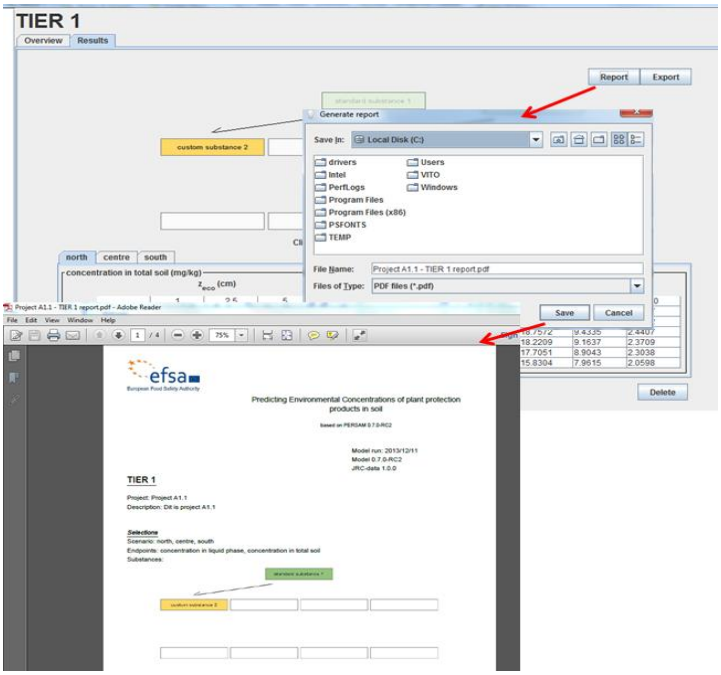

Figure 33: Generation of a pdf report for TIER-1

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10. Help

PERSAM contains a context sensitive help to assist the user easy comprehension. When the user clicks on the help, the help information corresponding to the current actions (f.i. calculation of TIER-1, …) will be shown.

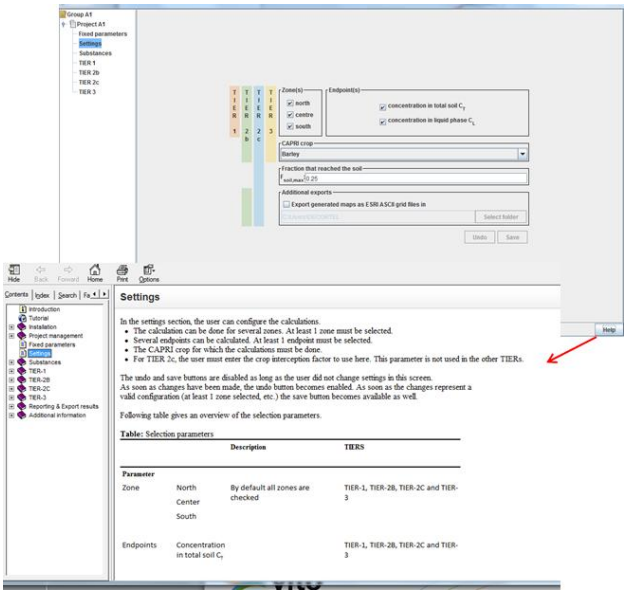

Figure 34: Help functionality

The PERSAM tool and the PERSAM user manual can be downloaded freely on the JRC soil portal (*http://eusoils.jrc.ec.europa.eu/library/Data/EFSA/).* The PERSAM user manual can also be downloaded on the EFSA website (*http://www.efsa.europa.eu/*) .

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

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

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

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APPENDICES

A. FUNCTIONAL REQUIREMENTS

Table 20: Functional requirements

Functional requirements	
Item	
Project management	✓ Organize projects in a tree structure ✓ Create, delete a group ✓ Modify an existing group (rename) ✓ Define a new project ✓ Open a project ✓ Modify and safe a project ✓ Import and export a project ✓ Copy and paste a project ✓ Remove a project
Substance management	✓ Configure a parent substance ✓ Define metabolites, up to 2 levels deep and up to 4 metabolites per level
Calculations	✓ TIER-1 PEC's: apply the analytical model on a single location; ✓ TIER-2B 95th-percentile PEC's: apply the analytical model in each 1km by 1km grid cell over Europe and extract the 95th-percentile of those values; and ✓ TIER-2C 95th-percentile PEC's using output from TIER-2A simulations with numerical models for the soil load including wash-off: adjust the output of TIER-2B by a user-provided correction factor. ✓ The tool must allow to select the grid cell including the scenario properties corresponding to the 95th-percentile PEC as needed for the scenario development of TIER-3: determine the location of the 1km by 1km grid cell where the output of TIER-2B can be found.
Reporting	✓ Display the results of the statistical analysis. ✓ Printing the results of the statistical analysis through the standard Windows printing interface. ✓ Save the results of the statistical analysis in pdf and csv format. ✓ The user must be able to copy text from the pdf report to paste it in other applications. ✓ The user must be able to save all the calculated maps in the ESRI ASCII format.
Various	✓ All the input and the output must be saved for later re-use ✓ All settings can be set to their defaults ✓ All used parameter values – the user-defined as well as the built in ones – must be visible to the user. ✓ Context sensitive help must be available

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B. NON-FUNCTIONAL REQUIREMENTS & QUALITY ATTRIBUTES

Table 21: Non-functional requirements & quality attributes

	Non-functional requirements & quality attributes
Item	
Installation and running	✓ Stand-alone application ✓ Running on Windows XP, Windows 7, and Windows 8, Windows 2008 server and later ✓ Freely downloadable from a website ✓ Installation of the software tool will not require additional software tools or applications ✓ The software should be installed by a self-contained installation package (auto-installing)
Scalability	✓ Modules implementing (to be developed) calculations for (to be developed) extra crops
Adaptability	✓ Incorporation of new map data (available from the JRC website) is possible. After incorporating new map data, the version number of the tool is increased.
Performance	✓ The calculations must complete within minutes.
Data	✓ The software uses the maps from the JRC-website
Security	✓ The source code and scenario properties used by the model should be protected against modifications/tampering by the user
Licensing	✓ No third party libraries subjected to license agreement constraints will be used

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C. CAPRI CROPS[6]

Crops
Barley
Common wheat
Dry pulses
Durum wheat
Floriculture
Maize
Oats
Other cereals
Other crops
Other fodder on arable land
Other non-permanent industrial crops
Other oilseed crops and fibre
Other root crops
Rape and turnip rape
Rye
Soybean
Sugar beet
Sunflower
Tobacco
Tomatoes and other fresh vegetables

Figure 35: Capri crops

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

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D. SOIL-SPECIFIC PARAMETERS[7]

Total concentration in soil

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

Concentration in liquid phase

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

[7] See Scientific opinion, EFSA 2012b

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E. SUBSTANCE-SPECIFIC PARAMETERS[8]

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

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

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

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ABBREVIATIONS

API	Application Programming Interface
CAPRI	Common Agricultural Policy Regionalised Impact model
CPU	Central Processing Unit
C_L	Liquid concentration in soil ($mg.L^{-1}$)
C_T	Total concentration in soil ($mg.kg^{-1}$)
DegT50	Half life for degradation in soil at 20°C (days)
DTO	Data Transfer Object
ρ	Dry bulk density ($kg.L^{-1}$)
EFSA	European Food Safety Authority
f_{om}	Organic matter content ($kg.kg^{-1}$)
$F_{soil,max}$	Fraction that reached the soil
GUI	Graphical User Interface
JCA	Java Cryptography Architecture
JPA	Java Persistence API
JRC	European Commission Joint Research Centre
K_{om}	Organic matter/water distribution coefficient ($L.kg^{-1}$)
MRLs	Maximum Residue Levels
NA	Not available
PEC	Predicted Environmental Concentration
PPP	Plant Protection Products
PU	Pesticides Unit
SAM	Simple Analytical Model
T_{Arit}	Arithmetic mean temperature (K)

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T_{Arr}	Arrhenius weighted average soil temperature (K)
TWA	Time weighted average
θ	Volumetric water content ($m^3.m^{-3}$)

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