



Project no. 022704 (SSP)

## FOOTPRINT

Functional Tools for Pesticide Risk Assessment and Management

Specific Targeted Research Project

Thematic Priority: Policy-orientated research

*Deliverable DL15*

**Software specification document for the three FOOT-Tools**

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| PP  | Restricted to other programme participants (including the Commission Services)        |   |
| RE  | Restricted to a group specified by the consortium (including the Commission Services) |   |
| CO  | Confidential, only for members of the consortium (including the Commission Services)  |   |

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## Foreword

This document was prepared within the context of work package WP5 ('Development of functional tools') of the FOOTPRINT project (<http://www.eu-footprint.org>). It presents software specification for the 3 tools which will be developed within FOOTPRINT.

Careful descriptions of the user requirements are the key to developing software efficiently that will be functional, useful and robust. This is critical to the design and development of software that must meet strict functionality and quality criteria. This document is sub-divided into three separate, but complementary, documents applicable to the FOOT-FS, FOOT-CRS and FOOT-NES systems. These software tools are being developed by an international consortium of European researchers as part of the FOOTPRINT (Functional tools for pesticide risk assessment and management) project (Project #022707) funded by the EU via the Sixth Framework Programme.

The documents detail how the individual parts of the three software systems will operate, interface and what facilities will be available to end users.

The preferred reference to this document is as follows:

Lewis K.A., Reichenberger S., François O., Bach M., and Dubus I.G. (2007). Software specification document for the three FOOT-tools. Report DL15 of the FP6 EU-funded FOOTPRINT project [[www.eu-footprint.org](http://www.eu-footprint.org)], 112p.



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## FOOTPRINT

Functional Tools for Pesticide Risk Assessment and Management

Specific Targeted Research Project

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**Software specification FOOT-FS – The farm scale tool**

Kathy Lewis

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# Software Requirements Specification Document

## FOOT-FS – The farm scale system

### Version 1.1 (February 2007)

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## Executive Summary

This document provides a software specification of the FOOT-FS (farm scale) tool. It details how the individual parts of the software, developed by different institutions within the consortium, will interface. It also provides a description of the purpose and functionality of the developed software.

FOOT-FS is mainly targeted at farmers and extension workers but has also relevance to many other groups. The tool will have the potential to help pesticide users develop crop protection strategies and help minimise losses of pesticides to the environment.

FOOT-FS will :

- Use a meta-modelling approach to predict environmental concentrations of pesticides in edge of field surface waters, abstraction points and groundwater. These data will then be compared with ecotoxicological end points for various aquatic fauna and flora to provide the risk assessment.
- identify the pathways and activities which most contribute towards contamination of water bodies.
- provide site-specific recommendations to limit transfers of pesticides to local agricultural landscapes.
- provide practical recommendations for reducing pesticide contamination of water resources.
- match the end report to the end users needs in terms of presentation style, content and depth of information.

FOOT-FS will be developed using Microsoft Visual basic 6.0 (with service pack 6) as the software language. Microsoft Access 2000 will be used for database development. Carbons Viewlet Builder will be used for help text and demonstration videos. User interfaces will be available in a range of European languages.

FOOT-FS will be developed as a collection of modules to be used sequentially. However, the system will also provide a 'user toolbox' which will include access to the FOOTPRINT Pesticide Properties Database and a version of MACRO unique to FOOTPRINT and a range of other tools. The system will be available as a stand alone software system and via a web portal.

The reliability and usability of the FOOT-FS tool will be assessed through a substantial programme of bench and beta testing, and of evaluation studies of the tool's predictive capability.

## **1 INTRODUCTION**

### **1.1 Purpose of this document**

Careful descriptions of the user requirements are the key to developing software efficiently that will be functional, useful and robust. This is critical to the design and development of software that must meet strict functionality and quality criteria. This document is applicable to the FOOT-FS system which is being developed by an international consortium of European researchers as part of the FOOTPRINT (Functional tools for pesticide risk assessment and management) project (Project #022707) funded by the EU via the Sixth Framework Programme.

This document will detail how the individual parts of the software will operate, interface and describes the facilities that will be available to end users. It will also provide a description of the purpose and functionality of the developed software.

As software development is an evolving process this document will develop as the project progresses such that, when the software is complete, it will also provide a record of the design and development process. Information on the revision of this document can be found in Section 8 'Document Management'.

### **1.2 Document scope**

This specification description applies to V1.0 of the software developed 2006-2008. It is intended for use by the research consortium to clarify the development process and to serve as a description of the development process undertaken for other interested parties. It is not intended that this document should provide guidance for end users.

### **1.3 Overview of FOOT-FS**

FOOT-FS is the FOOTPRINT farm-scale tool and is mainly intended for use by farmers and extension advisers. It aims to assist in the development of environmentally sound pesticide strategies for the farm by identifying the activities and pathways that most contribute to the contamination of water resources. It will also provide site-specific recommendations to limit transfers of pesticides in the local agricultural landscape.

FOOT-FS will be available in two formats. Firstly a stand-alone software system will be developed in Microsoft Visual Basic. A web portal to the system will also be developed. In addition both versions will be available in a range of European languages including English, French, Italian, German and Danish.

The stand-alone software tool itself will be a collection of modules that can be used independently of each other but collectively managed from within a simple software shell driven by navigation menus. This approach breaks the modelling and risk assessment process down into a number of discrete steps making it easier to use. The modules available will include:

A graphical and menu driven user interface to collect data from the user on their pesticide use, farm practices, landscape description and environmental characteristics (climate, soil etc). This information is then fed to the main model and calculation routines.

A graphical and menu reporting interface will deliver the risk assessment to the user in a format designed to match their needs. It will also deliver management and mitigation options designed to reduce pesticide contamination of water bodies.

A FOOT-FS toolbox will include a range of tools designed to support the end user. These will include multi-lingual facilities, support and guidance tools and database access.

More information can be found in Sections 4 and 5.

The web portal will take the form of a dedicated website. Users will be able to use screen menus to enter data building up pesticide programmes and agro-environment scenarios. Alternatively, it will be possible to download tools for data collection and upload data-files back to the website. The data will then be used remotely to perform the modelling calculations and interpret the data. The results and their interpretation will then be returned back to the user.

The classification of the agricultural land according to the pathways leading to contamination of water resources by pesticides will be based on a hybrid between the CORPEN and HOST methodologies. The prediction of pesticide concentrations in leaching and runoff/erosion will rely on the deterministic models MACRO and PRZM while simpler, more pragmatic, approaches (e.g. lookup tables and question/answer decision trees) will be used for assessing pesticide inputs via spray drift and point sources (storage places, farmyards). The predicted concentrations in surface water will then be used within risk assessment calculations for aquatic taxonomic groups such as fish, algae, invertebrates (e.g. Daphnia) and higher aquatic plants (e.g. Lemna) using ecotoxicological threshold values ('endpoints') stored within the FOOTPRINT PPDB.

## **2 GENERAL INFORMATION**

### **2.1 Primary function of FOOT-FS**

FOOT-FS is mainly targeted at extension services and farmers. However, it may also have applications with regulators, water managers and other stakeholders interested in investigating farm specific problems associated with the contamination of water bodies by the agricultural / horticultural use of pesticides.

The main aims of the tool are:

- i) The identification of the pathways and those areas that most contribute to contamination of water resources by pesticides at the scale of the farm.
- ii) To provide site-specific recommendations in order to limit transfers of pesticides in the local agricultural landscape.
- iii) To make practical recommendations for reducing pesticide contamination of water resources

### **2.2 Relationship to the other FOOT-tools (FOOT-CRS & FOOT-NES)**

As part of the FOOTPRINT project two other tools will be developed in parallel to FOOT-FS. These will function at the catchment / regional scale (FOOT-CRS) and National / European scale (FOOT-NES).

The three tools will have different end-user communities each having their own requirements and needs with respect to:

- System design
- User-interface
- Output presentation and interpretation.

Consequently the three tools will be physically distinct from each but share the same overall philosophy and underlying science. They will also share some of the same facilities and tools such as the FOOTPRINT PPDB. Therefore they will enable coherent and robust risk assessments of pesticide contamination of water bodies to be made at a range of scales relevant to management, mitigation and regulation.

### **2.3 Characterisation of end-users and their needs**

FOOT-FS end-users will range from farmers and their advisers to regulators and water managers. Each potential user group will have different needs with respect to system design, data input and

the presentation of model results. The computing skills of different potential end-users may vary considerably and it will be necessary to ensure that the user interface is sufficiently flexible in functionality to meet the needs of each group. Data input will need to be streamlined, efficient and simple to operate and the system output will need to be presented to the user in a format that is at an appropriate level of detail to match their needs.

### 2.3.1 Farmers and advisers

#### *User objectives:*

- To understand the landscape characteristics specific to the site which contribute to pesticide contamination of farm water bodies.
- To identify areas at risk.
- To identify farming practices and decisions that may increase the risk of pesticide pollution – both diffuse and point source.
- To identify mitigation processes which will help limit the transfer of pesticides to farm aquatic bodies.

#### *User limitations:*

- Potentially inexperienced in the use of computers and computer models.
- English may not be the users first language or it may not be spoken at all.
- Limited time availability and limited patience.
- Limited understanding of the underpinning science.
- May not have access to the Internet.
- Unlikely to be able to identify pesticide fate and ecotoxicological properties with out support and advice.
- Likely to be more familiar with pesticide brand names than the active substance constituents.

#### *User interface needs:*

- Simple and quick to operate.
- Graphical and menu driven.
- High level of user support and help.
- Available in a variety of EU languages.
- Tools for handling pesticide brands and providing access to pesticide properties.
- Fully operational on- and off-line.

#### *Results presentation requirements:*

- Minimal hard data.
- Significant help with interpretation.
- Practical guidance.

### 2.3.2 Regulators and water managers

#### *User objectives:*

- To identify the pathways and those areas that most contribute to the contamination of water resources by the agricultural use of pesticides.
- To identify farming practices and decisions that may increase the risk of pesticide pollution – both diffuse and point source.
- To identify mitigation processes which will help limit the transfer of pesticides to farm aquatic bodies.

#### *User limitations:*

- Likely to be more familiar with active substances than brands.
- May need support selecting pesticide properties.
- More sophisticated data input options for users with good computer skills.

*User interface needs:*

- Quick to operate.
- Moderate levels of user support and help.
- Tools for providing access to pesticide properties.

*Results presentation requirements:*

- Full access to model hard data.

### 3 SOFTWARE DEVELOPMENT

#### 3.1 Overview of development process

The development cycle that will be adopted for FOOT-FS is illustrated in Figure 1.

The System Specification document seeks to describe the purpose, functionality and the technical aspects of the tool including its objectives, end-users, programming language, system modules and data exchange. From this document a detailed design phase is undertaken that describes the system data flow, user interface (both data input and results output) and user facilities in terms of both their technical nature and end presentation. The software coding phase converts the scientific processes developed with the FOOTPRINT project into functional software. Databases will be developed and populated. Once the basic tool is developed it will under go extensive in-house bench testing before the beta versions are released for testing and workshop evaluations are undertaken. Finally, based on the outcomes and findings of the piloting and evaluation process the software is debugged, refined and polished.

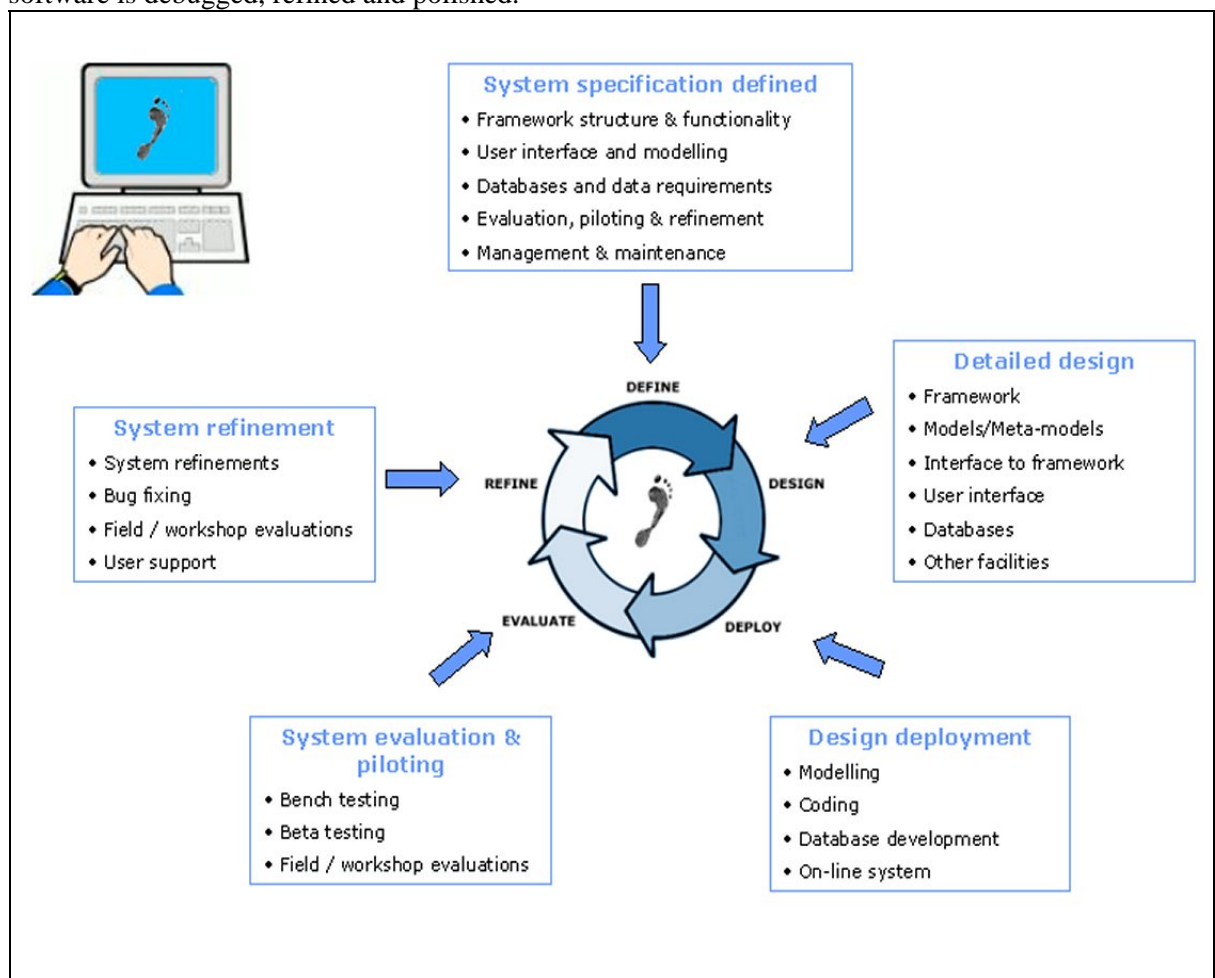


Figure 1: Schematic diagram of the FOOT-FS development cycle



## 3.2 Development languages, tools and platforms

### 3.2.1 Software

FOOT-FS will be developed using MICROSOFT (MS) Visual Basic Version 6.0 (with Service Pack 6) as the software language. Visual Basic (VB) is an event driven programming language and associated development environment created by Microsoft originally in 1991. VB enables Rapid Application Development (RAD) of graphical user interface (GUI) applications and easy access to databases using a variety of rapid data exchange techniques (e.g. DAO, RDO, or ADO).

Although Microsoft support for the VB6 development environment ceased in 2005, Microsoft still plans to offer mainstream development support for the VB6 runtime environment for the foreseeable future. This is anticipated to be through to the end of the Windows XP platform lifecycle (around six or seven years) and on into the Vista lifecycle (Vista is next version of Windows). Therefore it is not unreasonable to expect VB6 to be supported by Microsoft for at least another 10 years.

The VB6 development platform will be enhanced by the addition of a module designed to provide multi-lingual support. This is 'Multi-Language Add-In' available from Softwarebuero Jollans ([www.jollans.com](http://www.jollans.com)). This company develop software for technical applications such as VB and this tool provides a general solution for creating and maintaining multilingual versions of VB6 projects. The advantage of this approach is that just one version of the software is developed and translation of the strings is embedded into the software code. The module requires the software engineer to develop language dictionaries that holds the required language translations in all text used within the software program.

In addition to the main FOOT-FS software package a number of databases will be fully integrated and used for the storage and retrieval of meta-model data, agro-environment scenario descriptions, pesticide properties data and language dictionary elements

These will be developed and managed using Microsoft Access 2003 software package utilising the Access 2000 file structure. MS Access 2003 is a database-management system that allows you to create, edit, organise, store and retrieve database in a variety of different ways. This version of Access has been selected as it is robust and will support the Greek character set and fonts. Previous versions of Access, although accepting fonts and characters for most European languages they do not support Greek. Further information on the databases that will be integrated into FOOT-FS can be found in Section 6.1.

In order to enhance the user-help system, Qarbon's Viewlet Builder will be utilised within FOOT-FS ([www.qarbon.com](http://www.qarbon.com)). This software enables an animated slide show and tutorial of how to use the software to be created. The user can observe actual screen shots of the software in action, which is combined with on-screen annotation describing how to use the software. The animations are known as 'Viewlets' and are Flash based animations. An example can be seen in Figure 2.



Figure 2: Example of a simple annotated screen

### 3.2.2 Operating systems and hardware

FOOT-FS will be designed and developed to operate on both the Windows 2000 and Windows XP platforms. It is probable that the software will also work with Windows 98 and ME but Microsoft no longer support these systems.

The optimal and minimum hardware requirements for FOOT-FS will be identified during the System Performance bench testing exercises (see Section 7.3).

## 4 GENERAL FUNCTIONAL REQUIREMENTS

### 4.1 FOOT-FS shell

FOOT-FS will be developed as a collection of stand-alone modules. However, for operation on a PC an over-arching system shell will also be provided to help guide the user through the various stages of the risk assessment process. The shell will essentially be a Graphical User Interface that acts as a portal to the various modules.

The advantage of this approach is that it is memory efficient allowing the software to work on less powerful computers as only the module being operated is open and utilising computer memory at any one time. It also allows the risk assessment process to be carried out in stages rather than as a single exercise. It also enables easier and more efficient software maintenance.

### 4.2 What the system must accomplish

The system must:

- Meet the objectives of FOOT-FS (see Section 2.1).
- Harmonise with the other FOOT-tools (see Section 2.2)
- Meet the needs of all end-users in terms of functionality, performance and integrated user support (see Section 2.3).
- Be multi-lingual.
- Operate as a stand-alone software package and via a web-portal.
- Be maintainable and capable of being upgraded as simply and quickly as possible.

### 4.3 The system core and architecture

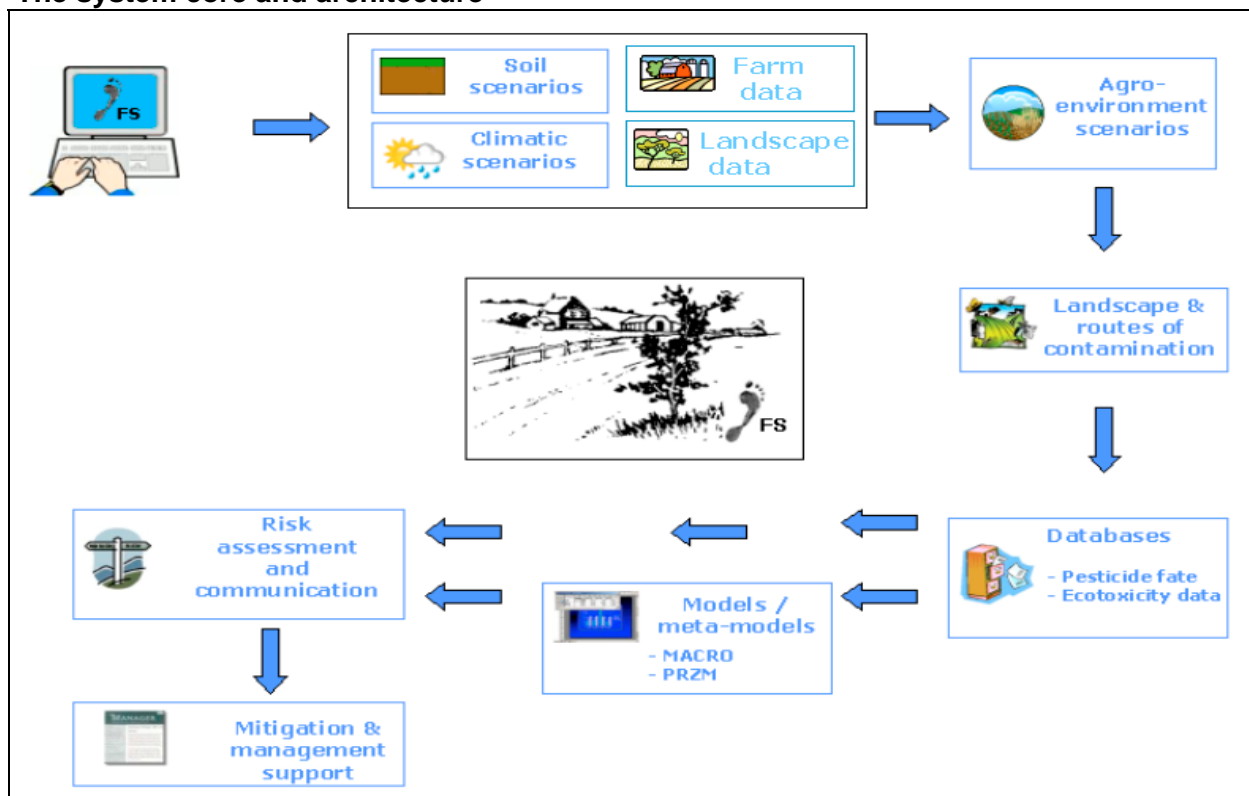


Figure 3: Schematic diagram of the FOOT-FS information flow

The schematic diagram above (Figure 3) shows the general flow of information through the FOOT-FS software.

- 1) The user must provide data to define their site in terms of soil, climate, farm cropping and landscape data (e.g. presence of water bodies such as ponds, ditches and streams and their location to the field being assessed). This will be possible either by selecting appropriate options from the pre-defined agro-environment scenarios or by entering data directly and the software system assigning the most appropriate scenario automatically. The user will also be required to input data on pesticide management practices in order to assess the risk of point source releases. This process will adopt a question and answer approach.
- 2) From the data provided by the user the software system will determine the probable routes of pesticide contamination of local water bodies. This will be achieved by the development of a flowchart decision tree based on the HOST/CORPEN methodology and will determine the models that will be used to calculate the predicted environmental concentrations.
- 3) The prediction of pesticide concentrations in leaching, runoff and erosion will rely on the meta-models derived from the deterministic models MACRO and PRZM driven by pesticide properties data taken from the FOOTPRINT PPDB (see Section 6.2). Simpler, more pragmatic, approaches (e.g. drift lookup tables) will be used for assessing pesticide inputs via spray drift. In addition, for more accomplished users, a version of the full MACRO model will also be available (See Section 6.3).
- 4) The predicted concentrations in surface water will be calculated and used within risk assessment calculations for a range of aquatic taxonomic groups such as fish, algae, invertebrates and higher plants using both acute and chronic ecotoxicological threshold values ('endpoints') stored within the FOOTPRINT PPDB where data is available. The calculation





will take into account the size and discharge of the water body as well as the volumes associated with runoff and drainage inputs and also the presence of bed sediment. The risk assessment process will use simple toxicity-exposure ratios.

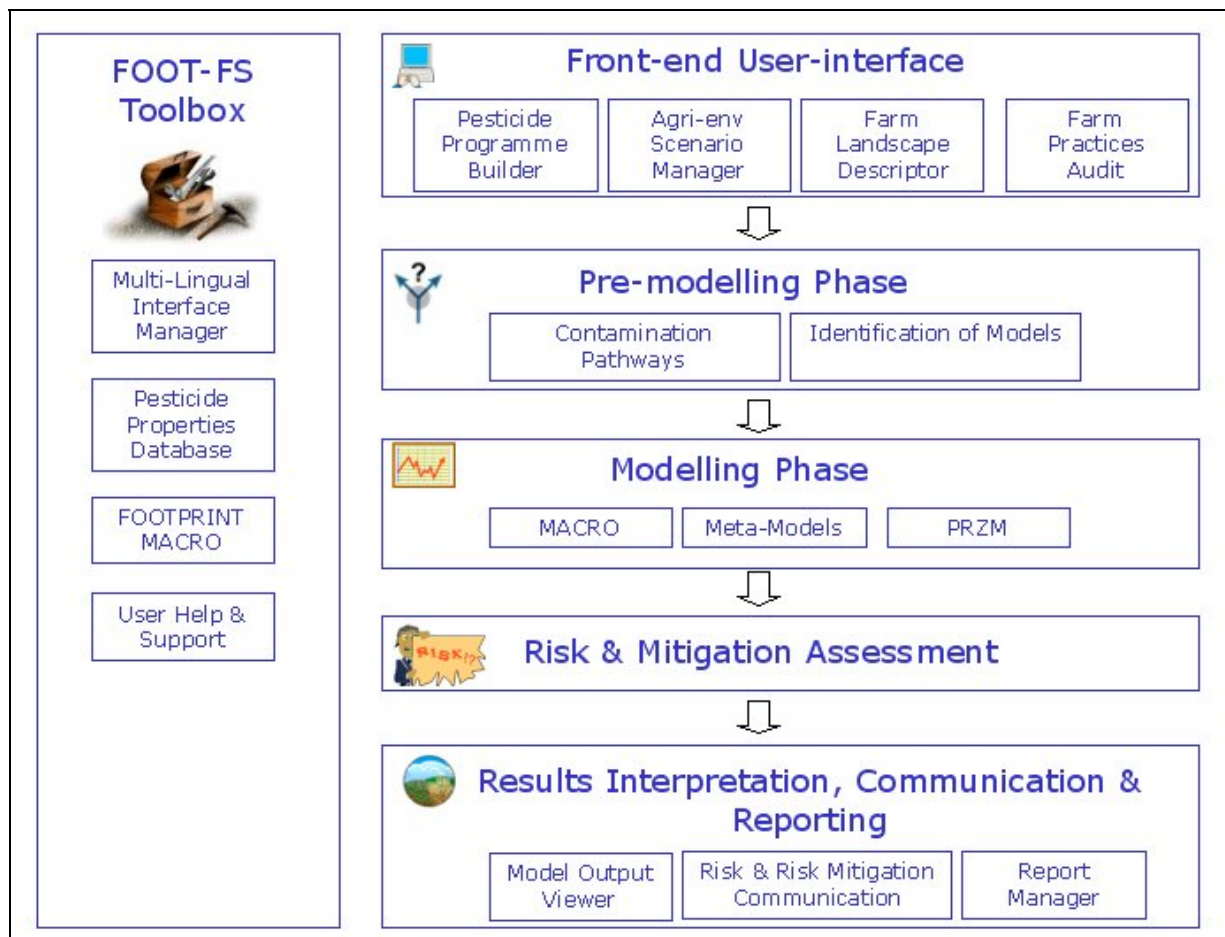
- 5) The use of mathematical models for assessing pesticide risk can generate significant amounts of numerical data that may need experience and some expertise to interpret. Therefore, for FOOT-FS consideration will need to be given to developing novel techniques and tools for communicating the risk to end users. These novel approaches may include scoring systems, graphical and icon representation or colour coding and will be used to identify high risk areas on the farm and aquatic fauna and flora that may be at risk. Such an approach will also be adopted for communicating the risk of point source releases from farm practices.

From this general description of the information flow through FOOT-FS it can be seen that the core elements of the software are:

- 1) Front end user-interface which must include:
  - Facilities for selecting agro-environmental scenarios or for collating data directly from the user and then automatically allocating the most appropriate agro-environmental scenarios.
  - Facilities for managing the input process – file management, editing, display and data validation.
- 2) Software routines for identifying pesticide contamination routes.
- 3) Pesticide properties database and user-interface.
- 4) Meta-models, the FOOTPRINT version of MACRO and risk calculations i.e. toxicity – exposure ratios.
- 5) Results communication user-interface which must include:
  - Full access to model output numerical data (predicted environmental concentrations, toxicity-exposure ratios) on demand for more experienced users but not as default.
  - Risk assessment communication module.
  - Management, pollution mitigation and risk abatement options.
  - Reports.
  - Output management facility – data and reports file storage, retrieval and display.

#### **4.4 The stand-alone system**

The stand-alone software tool itself will be a collection of modules that can be used independently of each other but collectively managed from within a simple software shell and operated by navigation menus. This approach breaks the modelling and risk assessment process down into a number of discrete steps making it easier to use and provides flexibility when re-using pesticide data with different scenarios and when exploring ‘what-if’ questions.



**Figure 4: Schematic diagram of the FOOT-FS system modules (Sections in blue are accessible and manageable by the user. Sections in black refer to the internal modelling and calculation routines).**

#### 4.4.1 The front-end user-interface

This module collates information from the user regarding the local site, environment and farm practices. This part of the system is visible to the end-user.

**Module 1:** Pesticide Programme Builder - this will allow pesticide strategies and application to be described, modified and saved in file format. These data files can then be read directly by Module 3. This module also includes the Brand Manager that allows data to be input by branded product rather than as active substance. See Section 5.2 for further information.

**Module 2:** Agri-environment Scenario Manager – this will allow the local site to be described by selecting soil, climate and agronomic scenarios to define the agro-environment of the farm. See Section 5.2 for further information.

**Module 3:** Farm Landscape Descriptor – this will collate information from the user about the on-farm water bodies. See Section 5.2 for further information.

**Module 4:** Farm Practices Audit – this will collate information from the user about pesticide handling and management activities using a question and answer approach to assess the risk of aquatic pollution from point source. See Section 5.2 for further information.



#### 4.4.2 The pre-modelling and modelling phases

These two modules are not accessible nor visible to the end-user.

Within the pre-modelling phase, decision rules will be used to identify the pesticide contamination pathways and identify the models that will be required. Data required to drive the meta-models and models will be identified and retrieved from the Pesticide Properties Database (See Section 6.2). The meta-models will then be used to calculate the pesticide leaching to groundwater and losses to surface water via drainage, drift, runoff and erosion.

#### 4.4.3 Risk assessment

This module is not accessible nor is it visible to the end-user. Using the results from the meta-modelling and modelling activities, the predicted environmental concentrations (PECs) in edge of field surface waters, surface water abstraction points and groundwater will be calculated and compared with ecotoxicological endpoints for various aquatic taxonomic groups to establish Toxicity Exposure Ratios (TERs) (See Section 5.4 for more information).

#### 4.4.4 Risk interpretation, communication and reporting

This module provides information to the user on the results of the risk assessment of diffuse releases.

**Module 1:** Model Output Viewer - this will allow all the model outputs, PECs and TERs to be viewed. It will also produce statistical summaries at application, crop, field and farm levels.

**Module 2:** Risk and Risk Mitigation communication. Risk communication provides the essential links between risk analysis, risk management, and the end-user. As the system could generate a large amount of data that would require interpretation, data visualisation and interpretation techniques will be used to describe the model results and convey complex scientific concepts in relatively simple terms.

**Module 3:** Report Manager – This module will allow the end user to create reports according to their specific requirements.

#### 4.4.5 FOOTPRINT Toolbox

In addition to the main FOOT-FS system a number of additional tools will be provided. These include:

**Multi-lingual interface:** The end-user will be provided with a choice of operating and reporting languages. These will include, for example: English, French, German, Italian, Danish and Polish.

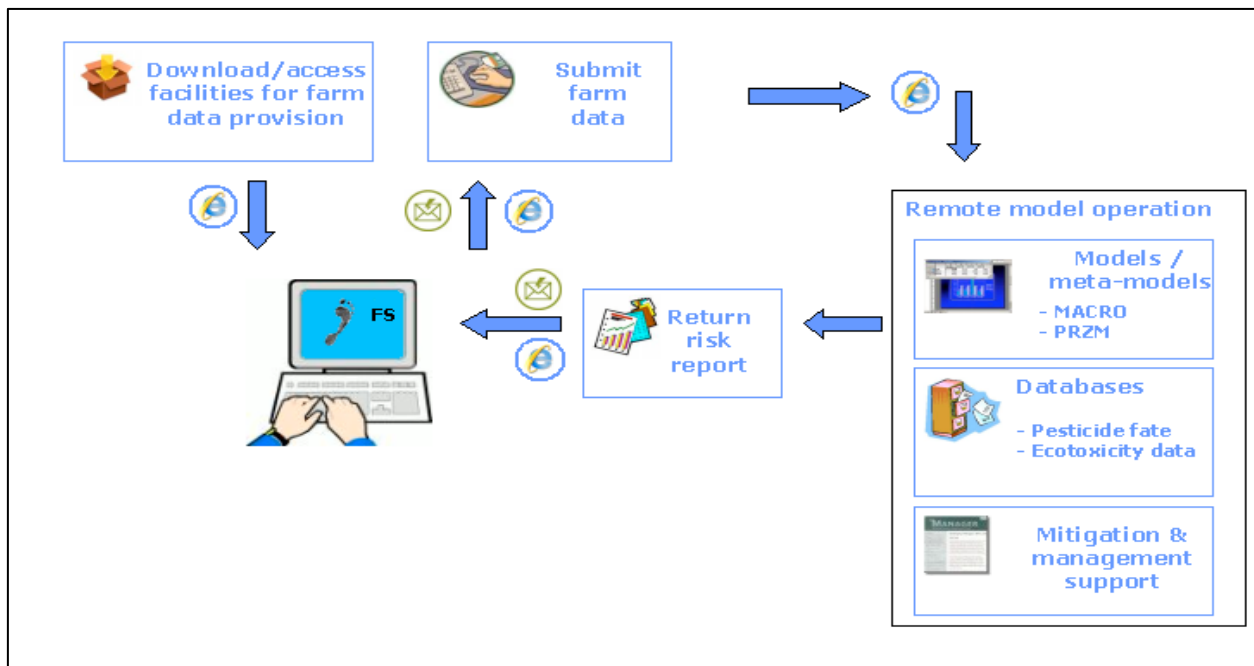
**Pesticide Properties Database:** An off-line version of the PPDB utilising a user-interface to the MS Access database similar to the version on-line (see Section 6.2) will be available. This will allow users to explore the data used to drive the meta-models and improve system transparency.

**FOOTPRINT MACRO:** For end-users not wishing to use the meta-models or agri-environmental scenario approach a full version of the MACRO model will also be available.

**User-support module:** A variety of help and support advice will be available at all levels of FOOT-FS. These will include:

- standard indexed help text and glossaries.
- user guide documentation in an electronic format.
- on-screen help.
- video-capture type presentations using the 'Show-Me' approach (also see Section 3.2).

## 4.5 The on-line approach



**Figure 5: Schematic diagram of the FOOT-FS online approach**

The on-line approach to be used with FOOT-FS will take the form of a web-portal offering remote operation.

Step 1: Users will access the FOOT-FS website and download tools to allow them to submit farm data. These tools will include the option to (a) download the Pesticide Programme Builder, Agri-environment Scenario Manager and Farm Landscape Descriptor (see Sections 4.3 and 5.2). (b) download interactive PDF/MS Word forms for entering the necessary farm data (c) accessing an online facility for data entry.

Step 2: Users return the data to the FOOT-FS website either by uploading forms and files or emailing them back directly.

Step 3: The user provided data is used to run the FOOT-FS system remotely. This process will be fully automated.

Step 4: System reports are returned to the user via email directly or by providing a link to a secure web page.

## 4.6 Software management

### 4.6.1 Bug fixing and software upgrades post release V1

A software bug is an error, failure, or fault in a software program that prevents it from behaving as intended. Bugs can arise from errors made during the program coding process and/or during its design. They can have a wide variety of effects, with varying levels of inconvenience to the user of the program. Serious bugs may cause a software program to stop operating i.e. to crash or to freeze. Usually these bugs will be identified during bench and beta testing exercises. However, some bugs may only occur in very specific circumstances or only with particular data sets. These usually have only a subtle effect on the program's functionality and so may lie undetected for a long time. It is virtually impossible to test and evaluate a software program's performance with every possible set of input data or in every possible way an end user may operate it. Consequently, it is rare for a software program to be completely bug free. Therefore it is important that procedures are put in place for end users to report bugs, for bugs to be fixed and upgrades or software patches distributed.



The FOOT-FS website will have facilities for users to report bugs directly to the software developers and to provide (wherever possible) the input data causing the problem. This is particularly important as it is not always easy to reproduce bugs. Some bugs are triggered by inputs to the program that may be difficult for the programmer to re-create.

Once the bug has been identified and fixed a corrected version of the module at fault will be available for download from the FOOT-FS website. Details regarding the error and bug fix will be also logged on the website. Each new release will be given a unique version number for reference.

#### 4.6.2 Software upgrades

From time to time it may be necessary for scientific or technical reasons to revise the software and/or the underpinning databases. If and when this occurs a new version of the module or modules revised will be available on the FOOT-FS website for download. Details of the upgrade, technical changes and release date will also be logged on the website. Each new release will be given a unique version number for reference.

## 5 THE CORE SYSTEM

### 5.1 System shell

The FOOT-FS system shell will operate only with the PC version. It will not be required for the on-line approach. It will include:

- Menu allowing the user to navigate through the modules to complete a risk assessment. Menu items will be direct links to the relevant modules and tools.
- Help and support including:
  - General introductory text to FOOT-FS, the other FOOTPRINT tools and the FOOTPRINT project.
  - General help text regarding the operation of the FOOT-FS system and the tools and facilities available.
- Links to relevant websites and online facilities (FOOT-FS online system, PPDB, FOOTPRINT website).
- Upgrading and updating tools showing module versions numbers, availability of upgrades and automatic upgrade functions.

### 5.2 Front-end user interface

As described previously there are three main modules for data input for FOOT-FS. Each module will be delivered as a stand-alone module that will function from a users computer hard drive. These modules will also be available for downloading from the FOOT-FS website as part of the on-line approach described in Section 4.5.

**Module 1: Pesticide Programme Builder.** This module provides the user with a facility to input data describing the pesticide applications to be evaluated by FOOT-FS. The facilities provided within this module will include:

- The ability to construct, name, save, retrieve, display, copy and edit different crop protection programmes using a menu-driven graphical interface approach will be provided. Data will include the pesticide applied (as active substance or brand – see below), application rate and application date. Data will be stored in an underpinning MS Access database so the user can return at a later time to modify programmes and applications, build new ones from existing applications or add new programmes and applications as required. Data validation procedures will be integrated into the software.
- A Pesticide Brand Manager will be included which is a simple tool to build up a database of pesticide brands. Each brand has a brand name, its formulation (liquid or solid), the active



substances it contains and the amount of the active substance(s) in the product in terms of grams per litre (g/l for liquids) or percent by weight (% w/w for solids). The user will be able to build up their own brands database, so that it only contains brands they use, or use a brands database that has been already compiled for, for example, a specific country. The advantage of having the brands database is that it saves the user time when creating applications in the Pesticide Programme Builder and will simplify data entry for farmers who will be more familiar with brands than active substances. Databases will be developed using MS Access. This tool will include functions for saving, retrieving, copying, editing and displaying the contents of the Bands database.

- User support facilities. See Sections 3.2 and 4.4.

**Module 2: Agri-environment Scenario Manager.** The FOOTPRINT project involves defining a large number of generic scenarios that characterise the complete spectrum of European agricultural environments. Each scenario will represent a unique combination of:

- **Cropping:** A list of crops of interest and templates for the critical crop growth stages required by the models to be used will also be derived.
- **Soil type:** A set of FOOTPRINT soil classes will be defined that have relatively homogeneous properties with respect to the required model soil variables. These will be based on two components: A hydrological one, which combines the characteristics used to derive the HOST and CORPEN conceptual models; a physico-chemical one which sub-divides each HOST/CORPEN soil grouping according to its textural, organic carbon and pH profile.

Data will be selected by entering spatial information defining the location of the site (e.g. longitude and latitude). This will then be used to identify the appropriate Soil Map Unit (SMU) as defined by the European Soil Database. The SMU will point to one or more FOOTPRINT Soil Types from which the user must select the most appropriate description for their site by responding to a small suite of questions. Should the user not accept the soil description matched to their inputs or if spatial data describing their location not available then a larger suite of questions will be available to provide an alternative route to identifying the FOOTPRINT Soil Type.

- **Climate:** A set of 15 FOOTPRINT climatic zones will be defined, within which the critical climatic variables that determine pesticide fate are relatively similar. The zone appropriate for the farm will be identified based on the same spatial information defining the location of the site as will be provided for identifying the FOOTPRINT Soil Type.

This module provides the user with the facility to identify the most appropriate pre-defined agri-environmental scenarios for their site. Once developed their descriptions and unique references will be stored using MS Access database. The user facilities will include:

- The ability to enter farm data into a graphical interface such that, using a suite of decision rules, the most appropriate agri-environmental scenarios are automatically identified. Options to save, retrieve, display and edit the data will be provided. Data validation procedures will be integrated into the software.
- The ability to select the most appropriate agri-environmental scenarios by describing the farm location in terms of, for example, map references. Again a graphical interface approach will be used. Options will be provided to save, retrieve and display the data.
- User support facilities. See Sections 3.2, 4.4 and 6.4.

**Module 3: Farm Landscape Descriptor.** This will collate information from the user about the on-farm water bodies such as their size, discharge and their location with respect to the fields where the pesticides are applied. Facilities will include:

- The ability to input the data using a menu-driven graphical interface. Options will be provided to save, retrieve, copy, edit and display the data.
- User support facilities. See Sections 3.2, 4.4 and 6.4.

**Module 4: Point Source Manager.** This module will use a qualitative approach to assessing farm activities and the risk of point source releases occurring. A Question and Answer type approach will be adopted with user responses linked to a decision tree and scoring system to assess risk.



Management issues will include waste handling of packaging, unwanted concentrates and unused solutions, filling and emptying of spray equipment, cleaning and maintenance of spray equipment. Facilities will include:

- The ability to input the data using a menu-driven graphical interface. Options will be provided to save, retrieve, copy, edit and display the data.
- User support facilities. See Sections 3.2, 4.4 and 6.4.

### 5.3 Pre-modelling phase and meta-modelling

Using farm data input into the system via the techniques described above together with a suite of decision rules the software will identify the pesticide contamination pathways and so identify the models that will be required. Data required to drive the metal-models and models will be identified and retrieved from the PPDB (see Section 6.2).

Mathematical modelling is the process of creating a mathematical representation of some scientific process in order to gain a better understanding of it. It is a process that attempts to match observation with a mathematical description. During the process of building the model, in order to simplify the mathematical representation, the developer must decide what factors are relevant to the problem and what factors can reasonably be ignored. The consideration and incorporation of more factors may well improve the models performance but this is often a trade-off against the models run-time and the computing power required for its operation. For scientists and regulators long model run-times may be acceptable but for the lay-person (e.g. farmers and their advisors) this may be prohibitive and is not desirable in farm management tools. To overcome this process a meta-model approach is to be taken for FOOT-FS. This requires model simulations (MACRO and PRZM) to be run for all the potential combinations of agro-environment scenarios developed (climate, soil, agronomic etc.) together with pesticide property data (pesticide sorption distribution coefficient Koc and soil dissipation half-life DT50).

The results from the meta-modelling exercises will then be formatted into look-up tables and stored as a suite of MS Access database files. Data from these will be retrieved based on the Koc and DT50 of the pesticide being modelled. The pesticide Koc and DT50 will be retrieved directly from the FOOTPRINT PPDB (see Section 6.2) although facilities will be incorporated to over-ride this default with the users own data.

As this part of the software is not within the control of the end user no user facilities or tools will be available.

### 5.4 Risk assessments

Using the results from the meta-modelling and modelling activities, the predicted environmental concentrations (PECs) in edge of field surface waters, surface water abstraction points and groundwater will be calculated. Concentrations will be estimated considering potential dilution effects based on the size, discharge of the water body, water volumes associated with runoff and drainage inputs and the presence of bed sediment.

Pesticide regulatory risk assessments for aquatic life are currently derived in the EU under Directive 91/414 EEC. This recommends a Toxicity-Exposure Ratio (TER) approach in which reasonable worst case toxicity data are compared with exposure data. A similar approach to risk assessment will be used within FOOT-FS. TERs will be calculated by comparing both acute and chronic ecotoxicological endpoints (where available) for fish, invertebrates, algae and higher water plants using data within the FOOTPRINT PPDB with the calculated PECs.

The following ecotoxicological end-points (Table 1) will be used in the first instance but where these are not available the closest match will be used.

| Taxonomic group | Preferred species   | Endpoint                        |
|-----------------|---|---------------------------------|
| Fish            | Rainbow trout ( <i>Oncorhynchus mykiss</i> ) or Bluegill sunfish ( <i>Lepomis macrochirus</i> ) | Acute 96-hour LC <sub>50</sub>  |
|                 |   | 21-day NOEC                     |
| Invertebrates   | Water flea ( <i>Daphnia major</i> or <i>Daphnia pulex</i> )                                     | Acute 48-hour ErC <sub>50</sub> |
|                 |   | 21-day NOEC                     |
| Algae           | Green algae ( <i>Selenastrum capricornutum</i> or <i>Scenedesmus subspicatus</i> )              | Acute 96-hour ErC <sub>50</sub> |
|                 |   | 96-hour NOEC                    |
| Higher plants   | Duckweed ( <i>Lemna major</i> or <i>Lemna minor</i> )   | 14-day EC <sub>50</sub>         |

**Table 1: Species and ecological endpoints used for risk assessment purposes.**

As this part of the software is not within the control of the end user no user facilities or tools will be available.

## 5.5 Results communication and reporting

A suite of decision rules will be used to interpret the calculated TERs and identify appropriate mitigation and management activities. As described previously this part of the system includes three modules.

**Module 1: Model Output Viewer.** This module will allow all the model outputs, PECs and TERs to be viewed. In addition, it will also produce statistical summaries at application, crop, field and farm levels. Options for data display will be available including graphical representations, on-screen tables and graphs. Facilities will be provided for users to save report files and retrieve and display them at a later date.

**Module 2: Risk and Risk Mitigation communication.** Risk communication provides the essential links between risk analysis, risk management, and the end-user. As the system could generate a large amount of data that would require interpretation, data visualisation and interpretation techniques will be used including colour-coding, icons, graphs, indexing and scoring approaches in order to draw attention to the areas on the farm presenting most risk. Data visualisation tools present information primarily through images rather than words. Data interpretation tools (such as indexes and scores) describe complex scientific concepts in relatively simple terms. Both of these tools can be particularly powerful in communicating information about environmental quality conditions (such as water quality) and ecotoxicological risks. Options will be provided enabling end users to select the type of data displayed and the display format.

**Module 3: Report Manager.** This module will allow the end user to create reports, customising them according to their specific requirements. Facilities will be provided to save, retrieve and display the reports generated.

## 6 ADDITIONAL FACILITIES

### 6.1 Pesticide Properties Database (PPDB)

The performance and reliability of mathematical models is ultimately governed by the quality of the model input data. Whilst there are a wide range of sources for the type of input data that will be required by FOOT-FS not all are of the highest quality and a certain amount of experience and understanding of the science driving the model is required to choose the best data available. The FOOTPRINT PPDB seeks to solve this problem by bring the best sources together in a





standardised electronic format. This database will be embedded into the FOOT-FS and FOOT-CRS software packages in MS Access 2000 format. The database will also be available online.

This database (FOOTPRINT PPDB) will be a comprehensive database of physicochemical and toxicological data relating to pesticide active substances. As the pesticide fate and risk models within the FOOT-tools will use the data in the database it is important that the data are of the highest quality possible. The best sources of information currently available are the monographs produced as part of the EU 91/414 review process. These documents will be the first choice for data but they are not available for all pesticides and so alternative sources of data will be used including national government resources, manufacturers, online databases and peer reviewed scientific publications.

Data sets will be cross-checked against each other as a means of ensuring data integrity. Where different sources of data have widely different values these will be validated by comparison with the original publications wherever possible. The database will be actively updated as additional information is identified and new and/or better data becomes available. Each data item will be 'tagged' with a code indicating the confidence the developers have in its quality. Confidence values will be in the range 5 (high) to 0 (low). A low value will not necessarily indicate that the data is incorrect but only that it can not or has not been validated. Confidence values will be based upon:

- The source of the data (e.g. EU dossier, manufacturer, other database or publication). Some existing data sets are no longer being maintained and updated. For example EU dossier data will acquire a confidence value of 5 where as estimated data may acquire a 0 or 1.
- The publication date of the data if known. Very old data may not have been determined using the same scientific procedures, standards and protocols used by the most recent investigations.
- Whether or not the data reference can be identified and used to cross check the data
- The match the data is to the desired parameter. For example the acute toxicity endpoint for fish required is the 96hr LC50 for Rainbow trout (*Oncorhynchus mykiss*) or Bluegill sunfish (*Lepomis macrochirus*). If an exact match can not be identified but data for a different species or a longer duration is available this will be used but the confidence score amended appropriately.
- A judgement on the fitness for purpose will also be made. For example dissipation data for European soils are preferred to those where conditions and soil types are very different.

The database will hold:

- General data describing the chemical such as its appearance, chemical structure and formula and in which EU States it is registered for use.
- Environmental fate data. For example the pesticide octanol-water partition coefficient (Log P), sorption distribution coefficient (Koc) and soil dissipation half-life (DT50).
- Ecotoxicological data. For example acute and chronic endpoint data for fish, aquatic invertebrates and aquatic plants.

## 6.2 Multi-lingual translations

As introduced in Section 3.2 the FOOT-FS software will be multi-lingual. This will be achieved using software development tools that handle the translation automatically at software run-time. However, to achieve this an electronic language dictionary is required. All strings used in the user-interface (including pesticide active substance common names) will be held in a MS Access database and referenced by an Identification Number (IN).

Against each Identification Number in the database the translations are held for each language. In the software development phase the Identification Number is held rather than the string itself. At run-time the Identification Number is automatically replaced by the appropriate string in the chosen language.



The following language translations are planned: English, French, German, Italian, Polish, Swedish, Danish, Greek and Slovenian. The integrity of the translations is being addressed by ensuring that the translation is carried out by the appropriate FOOTPRINT partner i.e. a native language speaker also fluent in English.

It is also anticipated that Spanish will be available. It is thought prudent to include Spanish due to the significant levels of pesticide use in Spain. However, as the FOOTPRINT consortium does not include a Spanish partner a translator will be required. This issue will also be addressed.

### 6.3 FOOTPRINT MACRO

MACRO is an established and evaluated physically-based one-dimensional numerical model of water flow and reactive solute transport in field soils. Where the FOOT-FS user feels that the pre-run meta-model scenarios are not suitable for his/her local conditions, a version of the full MACRO model will be available in the FOOT-FS toolbox. A Visual Basic Interface will be specially written for the FOOT-FS system, which will allow users to run their own scenarios, and save the results in a compatible format to the FOOTPRINT MS-Access databases containing pre-run meta-model results.

### 6.4 User help and support facilities

User support facilities will be embedded into the FOOT-FS software at all operational levels. All facilities will be available from the main menu of each module. The types of help that will be available will include:

- Standard indexed help text and glossaries. This will comprise of written descriptions of both the operational and technical aspects of FOOT-FS.
- The User Guide Documentation in an electronic format will be available for browsing.
- Screen by screen support providing guidance on data entry and data requirements.
- Video-capture type presentations using the 'Show-Me' approach (also see Section 3.2).

Help and support will be accessible to users via a variety of methods including:

- The main system menus of each software module and tools will provide access to the Indexed Help and glossaries.
- All data input and output screens will have Help buttons and Help icons. Help buttons will link users directly with specific Help text, bypassing the Help index. Help icons will be used to provide additional support such as explaining data input needs at a particular part of the software.
- Each part of the GUI's architecture (i.e. menus, data input boxes, buttons etc) will have associated 'tool-tips'. Tool-tips are used in conjunction with a cursor, usually a mouse pointer. The user hovers the cursor over an item, without clicking it, and a small box appears with the name or description of the item being hovered over.
- Video-capture 'Show-Me' presentations will be available for each software module accessible from the main-menu. As explained in Section 3.2 these presentations are comprised of an animated slide show/tutorial of how to use the software step-by-step. An example is given in Figure 6. (See also Figure 2 in Section 3.2)
- Mini 'Show-Me' presentations will also be available as down-loads from the FOOT-FS website as will the User Guide documentation.

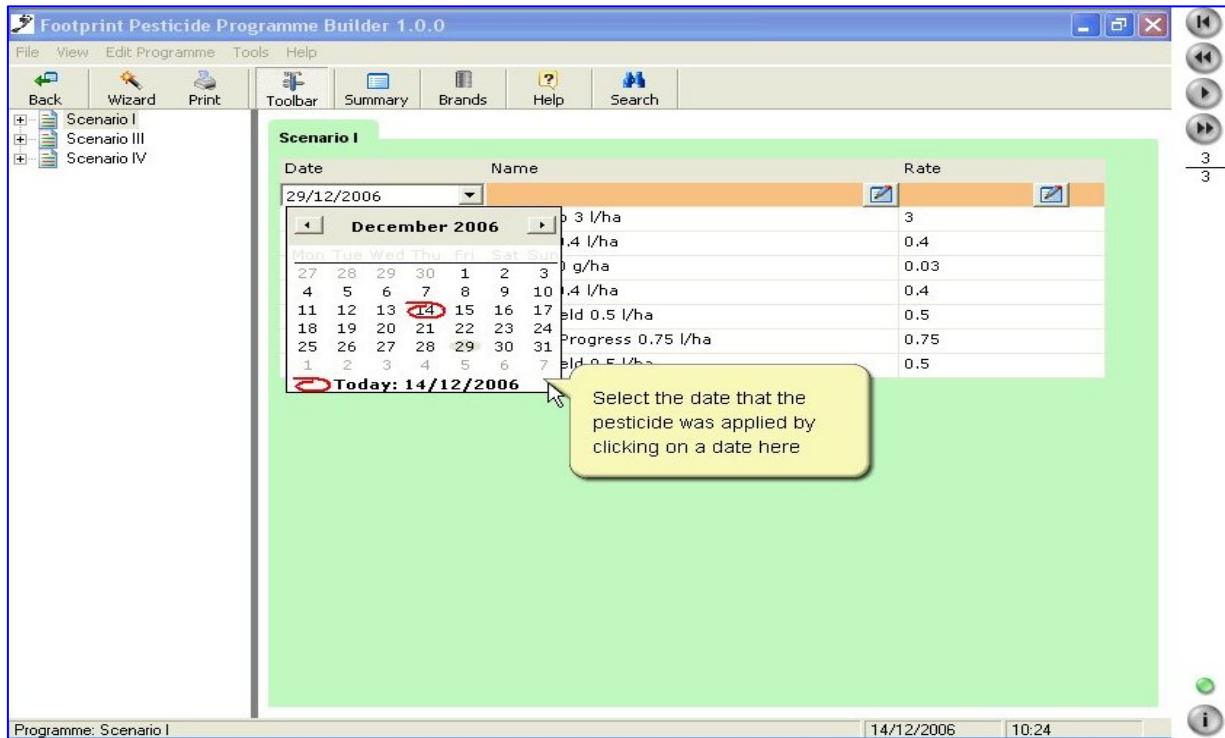


Figure 6: Example of a ‘Show-me’ screen providing user support with data input.

## 7 EVALUATION, REFINING AND POLISHING PROCESS

### 7.1 Evaluation

The reliability and usability of the FOOT-FS tool will be assessed through a substantial programme of piloting and evaluation tests at the bench, field, farm and small catchment scales, at sites representing a wide range of agro-environmental conditions in the EU. These will combine on-site evaluation as well as comparisons between tool predictions and monitoring data and/or alternative risk assessment methodologies.

Once the first draft of the software is completed a series of in-house bench testing exercises will identify and correct obvious bugs and usability short-comings. On completion a beta-version of the software will be available for piloting.

FOOT-FS will benefit from a piloting exercise where the usability and user-friendliness will be tested using a range of pilot farms in Sweden, France, the UK, Poland and Italy. Results of this piloting exercise will be fed back to the developers to improve the tools and to maximise its usability. The use of FOOT-FS will be subsequently evaluated in all countries represented on the consortium. Predictions from FOOT-FS will be compared to predictions of the stand-alone models (verification process) and to observed pesticide leaching in the field.

### 7.2 System refinement and software polishing

Feed-back from the piloting and evaluation tests will provide information on bugs, usability problems and system failures. These will be corrected and the system refined.

### 7.3 System performance evaluation

Software performance testing can serve different purposes. It can demonstrate that the system meets performance and/or functionality criteria. It can compare two systems to find which

performs or functions better. Or it can measure what parts of the system may cause the system to perform badly or fail. The earlier a performance defect is identified, the easier it is to correct. In all cases, it is often crucial for the test conditions to be similar to the expected actual end use.

Performance testing for FOOT-FS will be undertaken via in-house bench-testing and seek to achieve the following objectives:

- Verify input data collation time. Bench testing will identify typical data input times for users to verify that this is acceptable and to provide user guidance.
- Verify the system capacity versus model run-time. For example, the system could theoretically be used to assess all the pesticide applications made on all crops on all fields of a farm over a year or season. Performance testing will identify when the model run-time becomes unacceptable to end-users or when the data required or generated exceeds software or hardware capacity.
- Determine the optimal hardware/software configuration for FOOT-FS.
- Check that the data input routines have an adequate level of data validation.
- 

## 8 DOCUMENT MANAGEMENT

### Revision History

| <b>Date</b> | <b>Version</b> | <b>Description</b>          | <b>Author</b> |
|-------------|----------------|-----------------------------|---------------|
| 20/12/2006  | 1.0            | First draft of FOOT-FS SSD  | K A Lewis     |
| 27/02/2007  | 1.1            | Second draft of FOOT-FS SSD | K A Lewis     |
|             |                |                             |               |
|             |                |                             |               |

## 9 GLOSSARY

### 9.1 Abbreviations

| Abbreviation | Description  |
|--------------|--|
| ADO          | Microsoft ActiveX Data Objects   |
| DAO          | Microsoft Data Access Objects  |
| GUI          | Graphical User Interface   |
| MS           | Microsoft ®  |
| PDF          | Portable Document Format   |
| PEC          | Predicted Environmental Concentration  |
| PPDB         | FOOTPRINT Pesticide Properties Database  |
| RAD          | Rapid Application Development  |
| RDA          | Remote Data Access   |
| SSD          | Software Specification Document (NB SSD can also mean - Species Sensitivity Distribution. However, this meaning is not used within this document). |
| TER          | Toxicity-Exposure Ratio  |

### 9.2 Acronyms

| Acronym   | Description   |
|-----------|---|
| CORPEN    | Acronym - ‘Committee of ORientation for Practices Respectful of the ENvironment’<br>The CORPEN diagnostic methodology is widely used in France to characterise & mitigate the risk of pesticide transfers to groundwater and surface waters.  |
| FOOTPRINT | Functional Tools for Pesticide Risk Assessment and Management. EU funded Framework 6th Research project   |
| FOOT-FS   | FOOTPRINT – Farm Scale system   |
| FOOT-CRS  | FOOTPRINT – Catchment and Regional Scale system   |
| FOOT-NES  | FOOTPRINT – National and European Scale system  |
| HOST      | Acronym - ‘Hydrology Of Soil Types’<br>A delineation of UK soil types according to their hydrological properties to produce the 29-class Hydrology of Soil Types (HOST) classification. It is available as a 1km grid.  |
| MACRO     | Name relates to macropore flow.<br>MACRO is able to simulate tile drain outflow, leaching via preferential and matrix flow, decay, plant uptake, and foliar washoff of pesticides   |
| PRZM      | Acronym - (Pesticide Root Zone Model) PRZM is a one-dimensional, dynamic, compartmental finite-difference model that can be used to simulate chemical movement in unsaturated soil systems within and immediately below the root zone. The PRZM model is able to simulate surface runoff, erosion, chromatographic leaching, decay, plant uptake, foliar wash-off, and volatilisation of pesticides |



Project no. 022704 (SSP)

**FOOTPRINT**

**Functional Tools for Pesticide Risk Assessment and Management**

**Specific Targeted Research Project**

**Thematic Priority: Policy-orientated research**

***Deliverable DL15b***

**Software specification FOOT-CRS – The catchment and regional scale tool**

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| <b>Project co-funded by the European Commission within the Sixth Framework Programme (2002-2006)</b> |   |          |
| <b>Dissemination Level</b>   |   |          |
| <b>PU</b>  | Public  | <b>X</b> |
| <b>PP</b>  | Restricted to other programme participants (including the Commission Services)        |          |
| <b>RE</b>  | Restricted to a group specified by the consortium (including the Commission Services) |          |
| <b>CO</b>  | Confidential, only for members of the consortium (including the Commission Services)  |          |

# Software Requirements Specification Document

## FOOT-CRS – The catchment & regional scale system

### Version 1.1 (February 2007)

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## Executive Summary

This document provides a software specification of the FOOT-CRS (catchment and regional scale) tool. It details how the individual parts of the software, developed by different institutions within the consortium, will interface. It also provides a description of the purpose and functionality of the developed software.

FOOT-CRS is mainly targeted at water managers, local authorities and stewardship managers, but has also relevance to regulators and the crop protection industry.

FOOT-CRS will

- Identify those areas that most contribute to pollution of waters by pesticides.
- Define and optimise action plans for monitoring, mitigation and application restrictions etc at the catchment scale.

FOOT-CRS will be coded as an extension to the ArcGIS software by ESRI, and will be compatible to both ArcGIS 9.x and 10. FOOT-NES will be developed using MICROSOFT (MS) Visual Basic Version 6.0 (with Service Pack 6) as the software language, with Visual Studio 6 as the developing tool. Some scripts will also be developed in VBA as this permits easier development within ArcGIS. User interfaces will be available in English, French and German.

FOOT-CRS will be developed as a collection of modules to be used sequentially. The FOOT-CRS modules and functions will be accessible as menus in a dedicated toolbar in ArcMap.

The reliability and usability of the FOOT-CRS tool will be assessed through a substantial programme of bench and beta testing, and of evaluation studies of the predictive capability of the tool.



## **1 INTRODUCTION**

### **1.1 Purpose of this document**

Careful descriptions of the user requirements are the key to developing software efficiently that will be functional, useful and robust. This is critical to the design and development of software that must meet strict functionality and quality criteria. This document is applicable to the FOOT-CRS system (ArcGIS extension) which is being developed by an international consortium of European researchers as part of the FOOTPRINT (Functional tools for pesticide risk assessment and management) project (Project #022704) funded by the EU via the Sixth Framework Programme.

This document will detail how the individual parts of the software, developed by different institutions within the consortium, will interface. It will also provide a description of the purpose and functionality of the developed software.

As software development is an evolving process this document will develop as the project progresses such that, when the software is complete, it will also provide a record of the design and development process. Information on the revision of this document can be found in Section 8 'Document Management'.

### **1.2 Document scope**

This specification description applies to V1.0 of the software developed 2006-2008. It is intended for use by the research consortium to clarify the development process and to serve as a description of the development process undertaken for other interested parties. It is not intended that this document should provide guidance for end users.

## **2 GENERAL INFORMATION**

### **2.1 Primary function of FOOT-CRS**

FOOT-CRS is the catchment and regional-scale tool and will be available as an ArcGIS extension. FOOT-CRS is mainly targeted at water managers, local authorities and stewardship managers. However, it may also have applications with regulators or the crop protection industry, e.g. to investigate a region more closely when an application of the national and EU-scale tool FOOT-NES has identified this region as a potential "hot spot" of pesticide exposure.

The main objectives of the FOOT-CRS tool are to:

- identify those areas in a catchment or region that most contribute to pollution of waters by pesticides
- define and/or optimise action plans (monitoring, mitigation, application restrictions etc.) at the scale of the catchment.

The tool will contain two main parts with different outputs:

The "landscape analysis" part will provide a map showing the spatial distribution of the dominant pesticide contamination pathways (i.e. leaching, drainflow, runoff/ erosion, drift) in the catchment of concern. The classification of the agricultural land according to the pathways leading to contamination of water resources by pesticides will be based on remote sensing data (satellite imagery or aerial photos) and an adaptation of the HOST/CORPEN methodology used in the farm-scale tool FOOT-FS.

The "diagnostic" part will provide answers to the following questions:

- Where are the hot spots in the catchment?
- Is there a potential risk in the catchment for groundwater resources?
- Which mitigation measures must be implemented? Where? And to what extent, so that pesticide contamination of the water resources reaches an acceptable level?



Ultimately, with what frequency is a pesticide concentration of  $x \mu\text{g L}^{-1}$  in surface water (typically  $0.1 \mu\text{g L}^{-1}$ ) exceeded in a given period at the catchment outlet? Note that this a very ambitious target and it may turn out during the development of the tool that this is not feasible to achieve within this project.

The estimation of pesticide concentrations due to leaching, drainage and surface runoff/erosion will rely on the deterministic models MACRO and PRZM while simpler, more pragmatic approaches (e.g. drift calculation formulae according to FOCUS) will be used for assessing pesticide inputs via spray drift and point sources (storage places, farmyards). More details are given in chapters 4 and 5.

## 2.2 Relationship to the other FOOT tools (FOOT-FS and FOOT-NES)

As part of the FOOTPRINT project two other tools will be developed in parallel to FOOT-CRS. These will work at the farm scale (FOOT-FS) and National / EU scale (FOOT-NES). The three tools will be complementary and tailored to the different needs of the different user groups (cf. section 2.3). Redundant information or inconsistencies between the tools are therefore to be avoided. However, the three tools will share the same overall philosophy and underlying science, and also some facilities and auxiliary tools such as the FOOTPRINT PPDB.

While FOOT-FS and FOOT-NES will calculate Predicted Environmental Concentrations in surface water (PEC<sub>sw</sub>) for edge-of-field water bodies, the FOOT-CRS tool will calculate PEC<sub>sw</sub> at catchment outlets.

Both FOOT-CRS and FOOT-NES are conceived as ArcGIS extensions. The development of both tools shall be as close and harmonized as possible to ensure scientific and technical consistency. FOOT-CRS and FOOT-NES will share large parts of their code and their modular structure.

The range of mitigation measures included will be different for the three tools, corresponding to their different scales.

## 2.3 Characterisation of end-users and their needs

FOOT-CRS end-users will be predominantly local authorities, water managers and stewardship managers.

Each of these potential user groups will have different needs with respect to system design, data input and the presentation of model results. However, these needs will be less different than between the potential user groups of the farm-scale tool FOOT-FS. Computer literacy of different potential end-users may vary, but can be expected to be generally higher than for FOOT-FS users. It will be necessary to ensure that the user interface is sufficiently flexible in functionality to meet the needs of each group. Data input will need to be streamlined, efficient and simple to operate and the system output will need to be presented to the user in a format that is at an appropriate level of detail to match their needs. The possibility of errors due to wrong GIS handling has to be minimized.

### 2.3.1 Water managers, stewardship managers and local authorities

#### *User objectives:*

- To identify the pathways and those areas that most contribute to the contamination of water resources by the agricultural use of pesticides.
- To identify farming practices and decisions which may increase the risk of pesticide pollution.
- To identify mitigation strategies which will help limit the transfer of pesticides to surface water and groundwater bodies.
- To define and/or optimise action plans (monitoring, mitigation, application restrictions etc.) at the scale of the catchment, in order to ensure the necessary quality of drinking water for human consumption (legal drinking water limit of  $0.1 \mu\text{g L}^{-1}$  for a single active ingredient) or to comply with the Water Framework Directive.
- To play with what-if scenarios to assess the impact of climate change, changing agricultural policies etc.



#### *User limitations:*

- Not all users may be familiar with the use of GIS or remote sensing data.
- Not all users might be fluent in English (but fluency in either English, French or German can be anticipated).
- Likely to be more familiar with active substances than brands.
- May need support for selecting pesticide properties.
- More sophisticated data input options for users with good computer/GIS skills.

#### *User interface needs:*

- Quick to operate.
- integrate well into the ArcGIS user interface
- easy and safe replacement of default spatial data with better-resolved spatial data provided by the user
- Moderate levels of user support and help.
- Tools for providing access to pesticide properties.

#### *Results presentation requirements:*

- Full access to model hard data.
- Powerful export facilities (maps, reports, figures)
- Colour-coded output maps for communication with non-experts

## **2.4 What will FOOT-CRS do / not do?**

In the following, it will be discussed for different fields of application which purposes FOOT-CRS can or cannot be used for.

### **2.4.1 Mitigation**

FOOT-CRS will be able to assess the effect of given mitigation measures at the catchment scale. It will provide answers to the questions which mitigation measures must be implemented, where, and to what extent, in order to reduce pesticide contamination of water resources to an acceptable level. However, not all potentially effective mitigation measures can easily be effectively implemented in a real catchment. For instance, voluntary use restrictions for applying certain products in certain periods or recommendations for avoiding point sources may not be followed by farmers, or the installation of buffer strips or hedges may appear infeasible to economically pressed farmers. This cannot be considered in FOOT-CRS. However, to aid the successful communication of FOOT-CRS results from the user to farmers in the catchment, FOOT-CRS will provide convenient and flexible export facilities for maps and figures (cf. section 5.5).

### **2.4.2 Monitoring**

FOOT-CRS results will be usable to design and optimise monitoring networks, and also to select compounds to be analyzed during monitoring campaigns. However, it has to be kept in mind that the results of FOOT-CRS and any model cannot be better than the input data. If the inputs into the Pesticide Scenario Manager are poorly realistic due to lack of data on actual pesticide use, so will be the simulated pesticide concentrations at the catchment outlet.

### **2.4.3 Risk Assessment and Management**

FOOT-CRS will:

- calculate PEC<sub>sw</sub> at the catchment outlet
- calculate PEC<sub>gw</sub> in 1 m depth (regulatory-relevant depth)
- facilitate risk assessment for drinking water abstraction
- identify catchments with a high risk of pesticide contamination, e.g. due to vulnerable soils, high use of certain active ingredients, large areas of plant-protection-intensive crops etc.
- identify vulnerable catchments (i.e. catchments with a high potential risk of contamination due to soil, subsoil and climate characteristics)



- identify hot spots within catchments
- help to decide which activities should not be used at certain times, on certain areas or on certain crops
- produce output usable to communicate problem to farmers and advisors
- provide a starting point for more complex and data-hungry hydrological and hydrogeological models
- be able to perform both prospective and concrete-case exposure assessment

FOOT-CRS will NOT:

- calculate sharp pesticide concentrations in groundwater bodies. Instead, model results at 1 m depth will be considered together with groundwater vulnerability information (cf. Højberg et al., 2006) to identify areas with high risk for groundwater bodies.
- perform ecological risk assessment by comparing PEC<sub>sw</sub> with ecotoxicological thresholds

If only the FOOTPRINT default EU-wide spatial input data are available, FOOT-CRS should preferably not be used for risk assessment and risk management purposes in catchments where there is a known existing problem. In such cases, better resolved spatial data are necessary. However, for prospective assessments, the resolution of the EU-wide default data should usually be sufficient. Moreover, the scale of the assessment (i.e. the area of the catchment/region of interest) determines the necessary resolution of spatial input data. The smaller the catchment is, the higher resolved the spatial input data must be in order to obtain usable results.

#### 2.4.4 Point sources

It is acknowledged that point sources are an important input pathway for pesticides into water bodies and must be addressed. However, it turned out that at the catchment scale, there will most probably not be sufficient input data available to parameterize the HARDSPEC model (Hollis et al., 2004). Hence, point sources will be dealt with in an approximate, simple way.

#### 2.4.5 Kinetic sorption and bound residues

Kinetic sorption and bound residues will not be considered in FOOT-CRS. First, assessing the effects of formation and release of bound residues would require the use of the real MACRO model as opposed to the meta-model, and thus imply long calculation times. Second, the main user groups (water managers, stewardship managers, local authorities) will usually not have the necessary information to parameterize formation and release of bound residues for all soil/pesticide combinations occurring in a catchment.

#### 2.4.6 Uncertainty issues

The predictive capability of FOOT-CRS will be assessed in a number of evaluation studies with a range of test catchments, to establish credibility of the tool and its results (cf. section 7.1).

Each output of FOOT-CRS to the user will be accompanied with a qualitative or (where possible) quantitative statement of uncertainty. The limitations of the tool will be documented in the User Manual and mentioned in the FOOT-CRS output wherever necessary.

### 3 SOFTWARE DEVELOPMENT

#### 3.1 Overview of development process

The System Specification document seeks to describe the purpose, functionality and the technical aspects of the tool including its objectives, end-users, programming language, system modules and data exchange. From this document a detailed design phase is undertaken that describes the system data flow, user interface (both data input and results output) and user facilities in terms of both



their technical nature and end presentation. The software coding phase converts the scientific processes developed with the FOOTPRINT project into functional software. Databases will be developed and populated. Once the basic tool is developed it will under go extensive in-house bench testing before the beta versions are released for testing and workshop evaluations are undertaken. Finally, based on the outcomes and findings of the piloting and evaluation process the software is debugged, refined and polished.

## **3.2 Development languages, tools and platforms**

### **3.2.1 Software**

FOOT-CRS will be coded as an extension the the ArcGIS software by ESRI, and will be compatible with ArcGIS 9.x. The tool will use the Spatial Analyst extension of ArcGIS.

FOOT-CRS will be developed using MICROSOFT (MS) Visual Basic Version 6.0 (with Service Pack 6) as the software language, with Visual Studio 6 as the developing tool. Some scripts will also be developed in VBA that allows an easiest development within ArcGIS.

User interfaces will be available in English, French and German, which are the most widely used languages in the EU. The VB6 development platform will be enhanced by the addition of a module designed to provide multi-lingual support. This is 'Multi-Language Add-In' available from Softwarebuero Jollans ([www.jollans.com](http://www.jollans.com)). This company develops software for technical applications such as VB and this tool provides a general solution for creating and maintaining multilingual versions of VB6 projects. The advantage of this approach is that just one version of the software is developed and translation of the strings is embedded into the software code. The module requires the software engineer to develop language dictionaries that holds the required language translations in all text used within the software program.

In addition to the main FOOT-CRS software package a number of databases will be fully integrated and used for the storage and retrieval of meta-model data, agro-environment scenario descriptions, pesticide properties data (cf. section 6.1) and language dictionary elements (section 6.2). The same databases will be used for all 3 tools.

These will be developed and managed using Microsoft Access 2003 software package and the Access 2000 file structure.

### **3.2.2 Operating systems and hardware**

FOOT-CRS will be designed and developed to operate on both the Windows 2000 and Windows XP. Possibly the software will also work with older Windows versions, but only if ArcGIS actually runs on them.

The optimal and minimum hardware requirements for FOOT-CRS will be identified during the System Performance bench testing exercises (see Section 7.3).

## **4 GENERAL FUNCTIONAL REQUIREMENTS**

### **4.1 System shell**

FOOT-CRS will be developed as a collection of modules to be used sequentially. These modules will be accessible as menus in the ArcGIS Graphical User Interface.

The advantage of a modular approach is that is it memory efficient allowing the software to work on less powerful computers as only the module being operated is open and utilising computer memory at any one time. It also allows the risk assessment process to be carried out in stages rather than as a single exercise. It also enables easier and more efficient software maintenance.

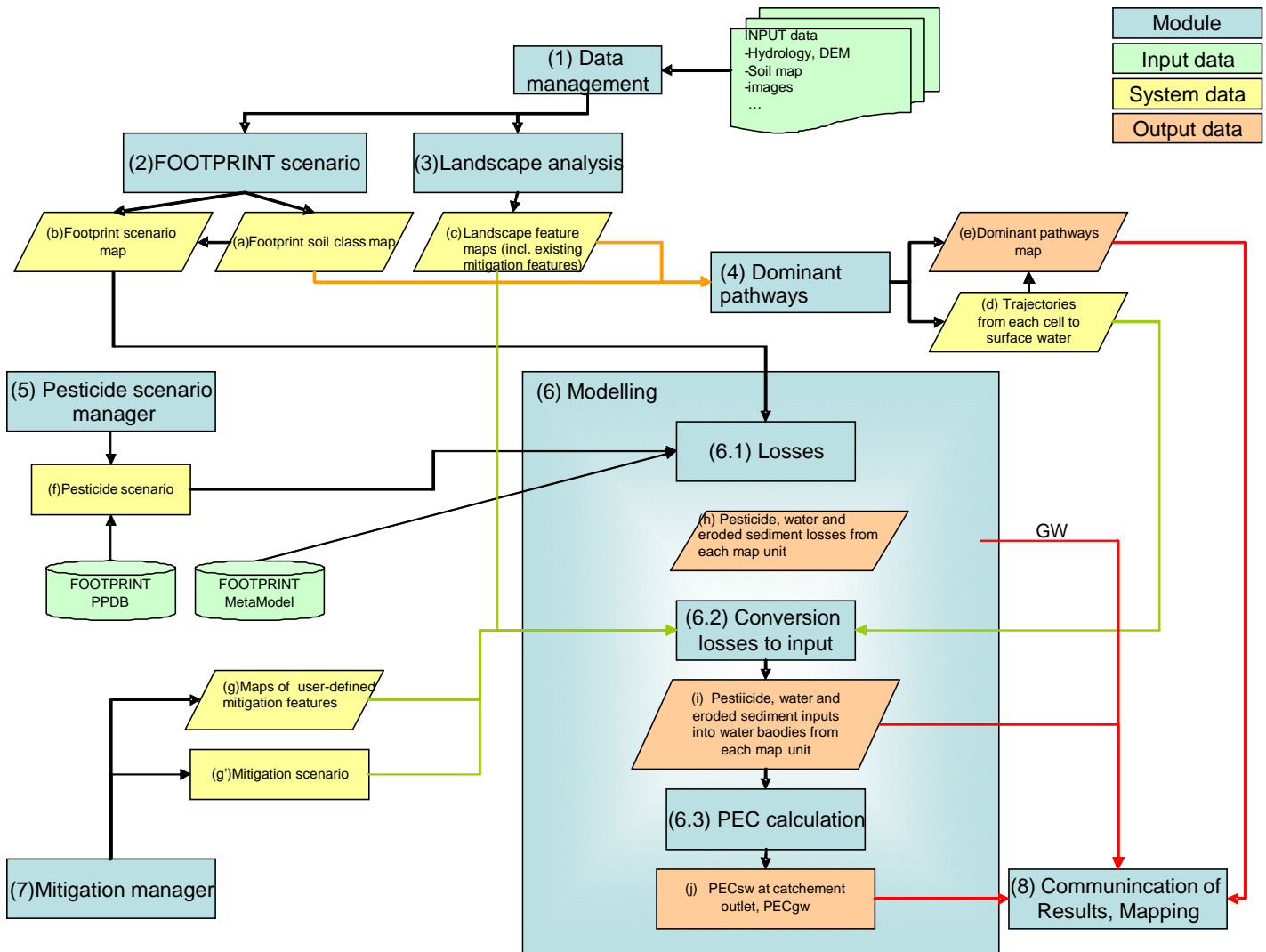
## 4.2 What the system must accomplish

The system must:

- Meet the objectives of FOOT-CRS (see Section 2.1).
- Harmonise with the other FOOT-tools (see Section 2.2)
- Integrate well with the ArcGIS software
- Meet the needs of all end-users in terms of functionality, performance and integrated user support (see Section 2.3).
- Be available in English, German and French.
- Be maintainable and capable of being upgraded as simply and quickly as possible.

## 4.3 The system core and architecture

The schematic diagram above (Figure 1) shows the general FOOT-CRS structure and flow of information. The software is broken down into 8 modules with different functions. A detailed tabular description of each module is given in Tables 1-8.



**Figure 1. Schematic diagram of the FOOT-CRS structure and information flow.**

**Explanations**

Manager: user interface that allows to add/modify/delete data (mainly geographic data)

System data: internal data; i.e. the user does not have direct access to them as opposed to input/output data.

- a) FOOTPRINT soil class map
- b) FOOTPRINT scenario map (FOOTPRINT “scenario” = FOOTPRINT agro-environmental scenario)
- c) Landscape feature maps
- d) Trajectories from each cell to surface water
- e) Dominant pathways map
- f) Pesticide scenarios (compound + application)
- g) Mitigation feature maps and g’: mitigation scenario.
- h) Maps of pesticide, water volume and eroded sediment losses from each map unit
- i) Maps of pesticide, water volume and eroded sediment inputs into water bodies from each map unit
- j) PECsw at catchment outlet and edge-of-field PECsw; PECgw



|                  |  |           |
|------------------|--|-----------|
| <b>Module</b>    | <b>Data management</b>   | <b>M1</b> |
| <b>Objective</b> | The user can manage the data layers of FOOT-CRS  |           |
| <b>Interface</b> | Data management window   |           |
| <b>Input</b>     | All default and user data (1)  |           |
| <b>Functions</b> | Import<br>Add/remove<br>Replace (to a certain extent)<br>Metadata description (source, scale...) |           |
| <b>Output</b>    | Dataset formatted in a usable way,<br>Data description in internal DB                            |           |

**Table 1a. The “Data Management” module.**

| (1) Dataset   | Geographic | Default  | Can be replaced by the user | Comments   |
|---|------------|--|-----------------------------|--|
| Soil map  | Yes        | European soil Data Base                        | Yes                         |  |
| DEM   | Yes        | SRTM   | Yes                         |  |
| Land cover  | Yes        | Corine land cover                              | Yes                         |  |
| Administrative boundaries   | Yes        | Nuts2 map                                      | Yes                         |  |
| Climatic scenarios  | Yes        | Grid from WP2                                  | NO                          |  |
| Surface water network   | Yes        | CCM2   | Yes                         |  |
| Catchment boundaries and outlet location                          | Yes        | CCM2   | Yes                         |  |
| daily discharge at the outlet                                     | Yes        | data from GRDC in Koblenz                      | Yes                         | either monthly means or Flow Duration Curves (FDC) |
| Layers used for GW vulnerability assessment                       | Yes        |  | Yes                         | TBD by Anker within WP2                            |
| Compounds DB  | No         | Footprint PPDB                                 | No                          |  |
| Metamodel DB  | No         | Footprint MM                                   | No                          |  |
| Drainage map (artificially drained percentage of the arable land) | Yes        | Estimate based on region and HOST-CORPEN class | Yes                         | To be done.  |
| Landscape features, see description in Module 3                   | Yes        | No   | Yes                         |  |

**Table 1b. Input data for FOOT-CRS.**

| <b>Module</b>              | <b>FOOTPRINT Scenario</b>   | <b>M2</b> |
|----------------------------|---|-----------|
| <b>Objective</b>           | Module that provides the map of FOOTPRINT soils classes and FOOTPRINT scenarios (either take default or facilitate map creation from user data)   |           |
| <b>Interface</b>           | Button “Create scenario map” in the main toolbar  |           |
| <b>Input</b>               | Soil maps, climatic scenario map, Area of Interest (Catchment boundary), DEM, Land use.<br>Scenario definition  |           |
| <b>Functions / actions</b> | Create FOOTPRINT scenario map (This will only be necessary if the user wants to use his own input data. The FOOTPRINT default scenario maps will have been created beforehand and will be included in the software CD/DVD.) |           |
| <b>Output</b>              | Map of FOOTPRINT soil Classes<br>Map of FOOTPRINT Scenario  |           |

**Table 2. The “FOOTPRINT Scenario” module.**

|                            | <b>Landscape analysis</b>   | <b>M3</b> |
|----------------------------|---|-----------|
| <b>Objective</b>           | Import or create the landscape feature maps from image analysis.  |           |
| <b>Interface</b>           | <ul style="list-style-type: none"> <li>- Dedicated tool bar (TBD)</li> </ul>  |           |
| <b>Input</b>               | <ul style="list-style-type: none"> <li>- (aerial or satellite) Imagery</li> <li>- Any vector layer</li> <li>- Catalog of reference images.</li> </ul>   |           |
| <b>Functions / actions</b> | <p>The Landscape feature layer can be</p> <ul style="list-style-type: none"> <li>- either a land cover-like map i.e. the whole area of interest is described, and each polygon has attributes that describe the type and density of features,</li> <li>- or a map of individual features, each feature being represented by a polygon and attributes describing the type of feature (grass strip, low/high hedges..).</li> </ul> <p>In the first case, the user will have to identify some landscape areas by Computer-assisted photo-interpretation using reference photographs / satellite images and graphics. He will have the opportunity to assign a set of properties from his interpretation of imagery.</p> <p>In the second case, he will have to delineate the features one by one. Some semi-automatic tool will be proposed to initiate the layer from the available image.</p> <p>(series of actions)</p> <ul style="list-style-type: none"> <li>- Add new Landscape feature map (option : blank layer or from existing vector data, i.e. CORINE Land Cover)</li> <li>- Edit Landscape feature map : vector and attributes</li> <li>- Save</li> <li>- Display reference catalog</li> <li>- Classify image using reference area</li> <li>- Image to vector.</li> </ul> |           |
| <b>Output</b>              | <ul style="list-style-type: none"> <li>- Landscape feature layers</li> </ul>  |           |

**Table 3. The “Landscape Analysis” module.**

| Module                     | Dominant pathways  | M4 |
|----------------------------|--|----|
| <b>Objective</b>           | <p>Create the dominant pathways map. The map of dominant pathways will state whether an area is more likely to pesticide losses via surface runoff/erosion, drainflow, drift or leaching.</p> <p>Create trajectories to nearest surface water body</p>   |    |
| <b>Interface</b>           | Button “Create dominant pathways map” in the main toolbar  |    |
| <b>Input</b>               | <p>Footprint soil classes map, landscape features map, DEM and surface water network</p> <p>Decision rules from WP3</p>  |    |
| <b>Functions / actions</b> | <p>Create dominant contamination pathways map (again DEM cells as map units).</p> <p>Calculate trajectories from each map unit (= DEM cell) to the nearest surface water body/bodies (runoff: downhill flowpath using DEM; drift: straight lines in 8 directions (N, NE, E, SE, S, SW, W, NW)?</p> |    |
| <b>Output</b>              | <p>Map of dominant contamination pathways</p> <p>Trajectories from each map unit to the nearest sw body, separately for surface runoff and drift (no map output to user; only internal use)</p>  |    |

**Table 4. The “Dominant Pathways” module.**

| Module                     | Pesticide scenario manager   | M5 |
|----------------------------|--|----|
| <b>Objective</b>           | Allows the user to define and manage the pesticide scenario  |    |
| <b>Interface</b>           | Pesticide scenario window  |    |
| <b>Input</b>               | <ul style="list-style-type: none"> <li>- Footprint Crop list</li> <li>- Footprint PPDB</li> </ul>  |    |
| <b>Functions / actions</b> | <p>User input of the following parameters.</p> <ul style="list-style-type: none"> <li>- active substance (select from PPDB or enter own DT50/Koc)</li> <li>- crop</li> <li>- application date</li> <li>- application rate</li> <li>- % of crop treated</li> </ul> <p>Possibility to apply pesticide to more than one crop; then repeat steps above for the other crops.</p> <p>Option 1: Unique parameter values for the whole AOI, then the user select a value in a combo-box for each parameter.</p> <p>Option 2 : For some parameter (e.g. application rate, application month, % of crop treated), the value can be localized. For each parameter, the user can:</p> <ul style="list-style-type: none"> <li>- Create a new “&lt;parameter&gt; map”, from an existing Vector layer</li> <li>- assign a &lt;parameter&gt; value to each polygon. (from an predefined list of choice)</li> </ul> <p>The user can manage (new, save, modify, delete) the scenarios.</p> |    |
| <b>Output</b>              | <p>Pesticide scenarios list in DB</p> <p>Parameters of each scenario in DB</p>   |    |

**Table 5. The “Pesticide Scenario Manager” module.**

| Module                     | Modelling   | M6 |
|----------------------------|---|----|
| <b>Objective</b>           | Compute PEC maps and PEC (or any other variable TBD) at the outlet.   |    |
| <b>Interface</b>           | “Perform Model” button  |    |
| <b>Input</b>               | <ul style="list-style-type: none"> <li>- Water network, outlet localisation, discharge, ...</li> <li>- Data for GW vulnerability assessment (TBD by Anker)</li> <li>- Footprint scenario map</li> <li>- Pesticide scenario</li> <li>- Metamodel DB</li> <li>- Mitigation scenario (none by default)</li> <li>- Modelling algorithm</li> </ul> |    |
| <b>Functions / actions</b> | The user can select a Mitigation scenario. By default, no mitigation scenario is selected.<br>Modules 6.1, 6.2, 6.3 are run successively.   |    |
| <b>Output</b>              | Pesticide input maps for each pathway<br>Results tables/figures at the outlet (e.g. CDF).   |    |

**Table 6a. The “Modelling” module**

| Module                     | Losses modelling  | M6.1 |
|----------------------------|---|------|
| <b>Objective</b>           | Compute pesticide, water and sediment losses  |      |
| <b>Interface</b>           | “Perform Model” button  |      |
| <b>Input</b>               | <ul style="list-style-type: none"> <li>- Footprint scenario map</li> <li>- Pesticide scenario</li> <li>- Metamodel DB</li> <li>- Mitigation scenario (none by default)</li> </ul> |      |
| <b>Functions / actions</b> | For each mapping unit and contamination pathway, compute the pesticide losses (if applicable, also water and eroded sediment losses).   |      |
| <b>Output</b>              | <ul style="list-style-type: none"> <li>- Maps of pesticide, water and eroded sediments losses from each map unit</li> <li>- Map of PECgw in 1 m depth</li> </ul>                  |      |

**Table 6b. The “Losses Modelling” sub-module.**

| Module                     | Losses conversion to inputs   | M6.2 |
|----------------------------|---|------|
| <b>Objective</b>           | Compute pesticide, water and eroded sediments inputs into water bodies from each map unit   |      |
| <b>Interface</b>           | - none -  |      |
| <b>Input</b>               | <ul style="list-style-type: none"> <li>- Water network</li> <li>- Maps of pesticide losses</li> <li>- Map of losses of water volume and sediment</li> <li>- Trajectories from each cell to surface water</li> <li>- Landscape features</li> <li>- Mitigation scenario (none by default)</li> <li>- Data for GW vulnerability assessment (TBD by Anker)</li> </ul> |      |
| <b>Functions / actions</b> | For each pathway and mapping unit, convert losses from the unit to inputs into water bodies.  |      |
| <b>Output</b>              | Maps of pesticide, water and eroded sediments inputs into water bodies from each map unit.<br>Maps of pesticide concentrations in groundwater.  |      |

**Table 6c. The “Losses Conversion To Inputs” sub-module.**



|                            |  |             |
|----------------------------|--|-------------|
| <b>Module</b>              | <b>PECsw computation</b>   | <b>M6.3</b> |
| <b>Objective</b>           | Compute PECsw at the catchment outlet.   |             |
| <b>Interface</b>           | - none -   |             |
| <b>Input</b>               | <ul style="list-style-type: none"> <li>- Surface water network, outlet localisation, discharge, ...</li> <li>- Maps of pesticide, water and eroded sediments inputs into water bodies from each map</li> </ul> |             |
| <b>Functions / actions</b> | TBD  |             |
| <b>Output</b>              | Results tables/figures at the outlet (e.g. CDF).   |             |

**Table 6d. The “PECsw Computation” sub-module**

|                            |  |           |
|----------------------------|--|-----------|
| <b>Module</b>              | <b>Mitigation manager</b>  | <b>M7</b> |
| <b>Objective</b>           | Allows the user to define and manage the mitigation scenario   |           |
| <b>Interface</b>           | Mitigation manager window  |           |
| <b>Input</b>               | List of predefined mitigation measures and associated predefined parameters (these are the parameters that define the mitigation action. For instance, if the mitigation strategy is “reduction of application rate”, then “% of reduction” or “Alternative application rate” is the associated parameter.   |           |
| <b>Functions / actions</b> | <p>Some mitigation measures are “global”, e.g. change of the application date or rate. (The user chooses the nominal pesticide scenario in the Pesticide scenario Manager, and computes the results. Then he can add some mitigation measures and run the model again. The results of the simulation with mitigation measures are then compared with those of the nominal pesticide scenario).</p> <p>Some measures can be localized (e.g. buffer zones).</p> <p>The mitigation manager allows the user to define and save different mitigation scenarios.</p> |           |
| <b>Output</b>              | <p>Mitigation scenarios list in DB</p> <p>Parameters of each mitigation scenario in DB.</p>  |           |

**Table 7. The “Mitigation Manager” module.**

|                            |   |           |
|----------------------------|---|-----------|
| <b>Module</b>              | <b>Display + Mapping of Results</b>   | <b>M8</b> |
| <b>Objective</b>           | Display results (maps and figures)  |           |
| <b>Interface</b>           | ArcGIS main window with dedicated legend button<br>Modelling result window.   |           |
| <b>Input</b>               | <p>Maps from module 2, 4, and 6</p> <p>Figures from module 6</p>  |           |
| <b>Functions / actions</b> | <ul style="list-style-type: none"> <li>- The user can</li> <li>- Display PEC maps (for each pathway), and change legend</li> <li>- Display figures (+explanatory text) from the modelling (e.g. CDF)</li> <li>- Display summary text (report).</li> <li>- Display proposed mitigation strategies</li> <li>- Export maps and reports.</li> </ul> |           |
| <b>Output</b>              | <ul style="list-style-type: none"> <li>- Result display</li> <li>- Exports (maps/figures as jpg/pdf; report as txt/doc/pdf)</li> </ul>  |           |

**Table 8. The “Display + Mapping of Results” module.**

#### 4.4 Integration in ArcGIS and graphical user interface

The FOOT-CRS modules and functions will be accessible as menus in a dedicated toolbar in ArcMap.

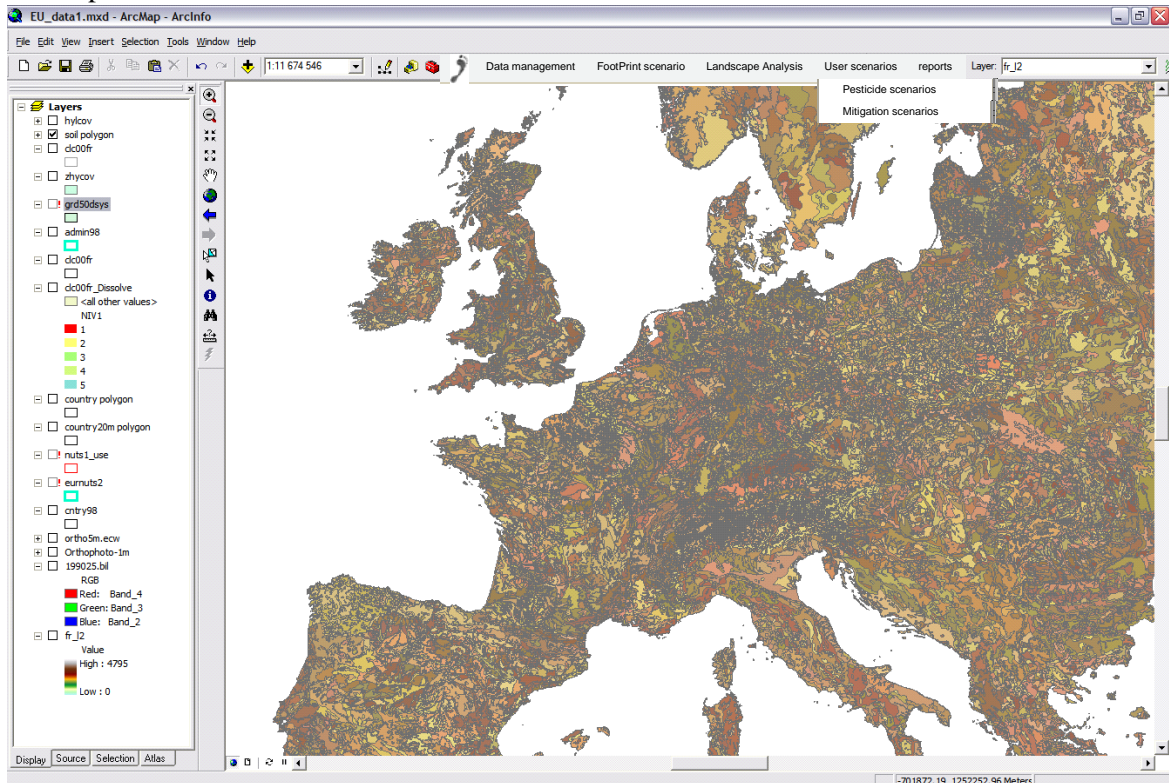


Figure 2. FOOT-CRS toolbar in ArcMap

The main graphical user interface (GUI) are presented in the next figures. They are all independent windows opened on top of the ArcMap window.

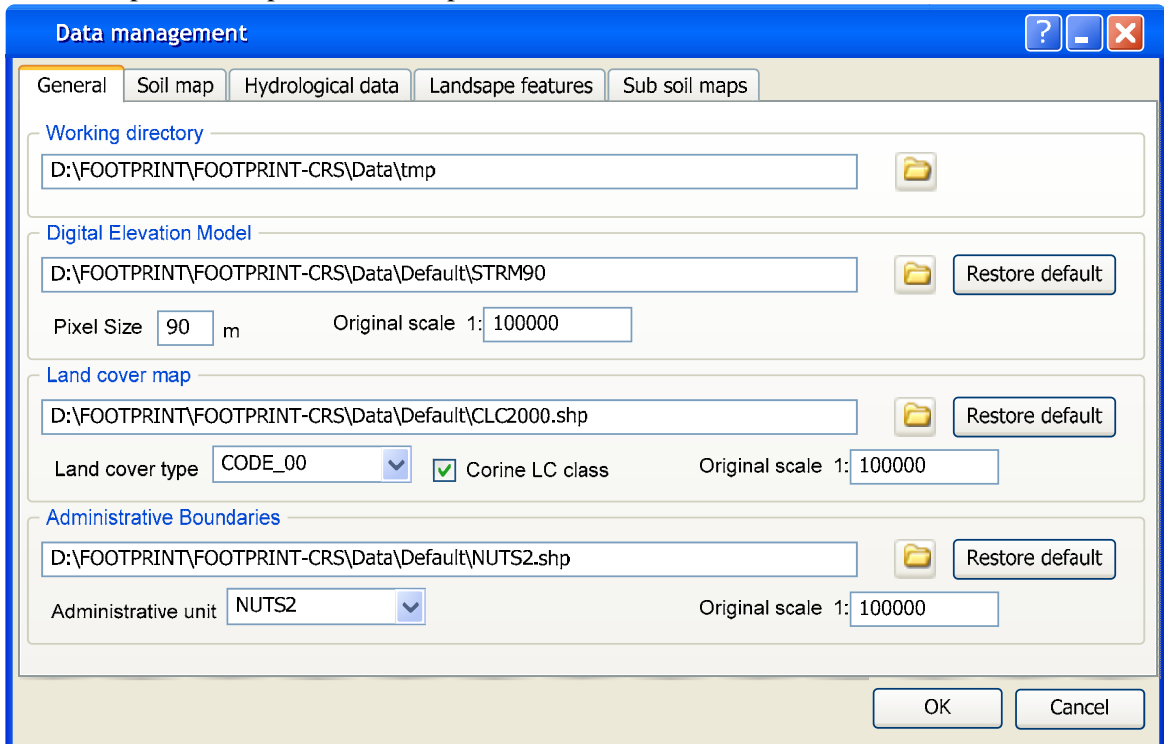


Figure 3a. FOOT-CRS Data management GUI – General

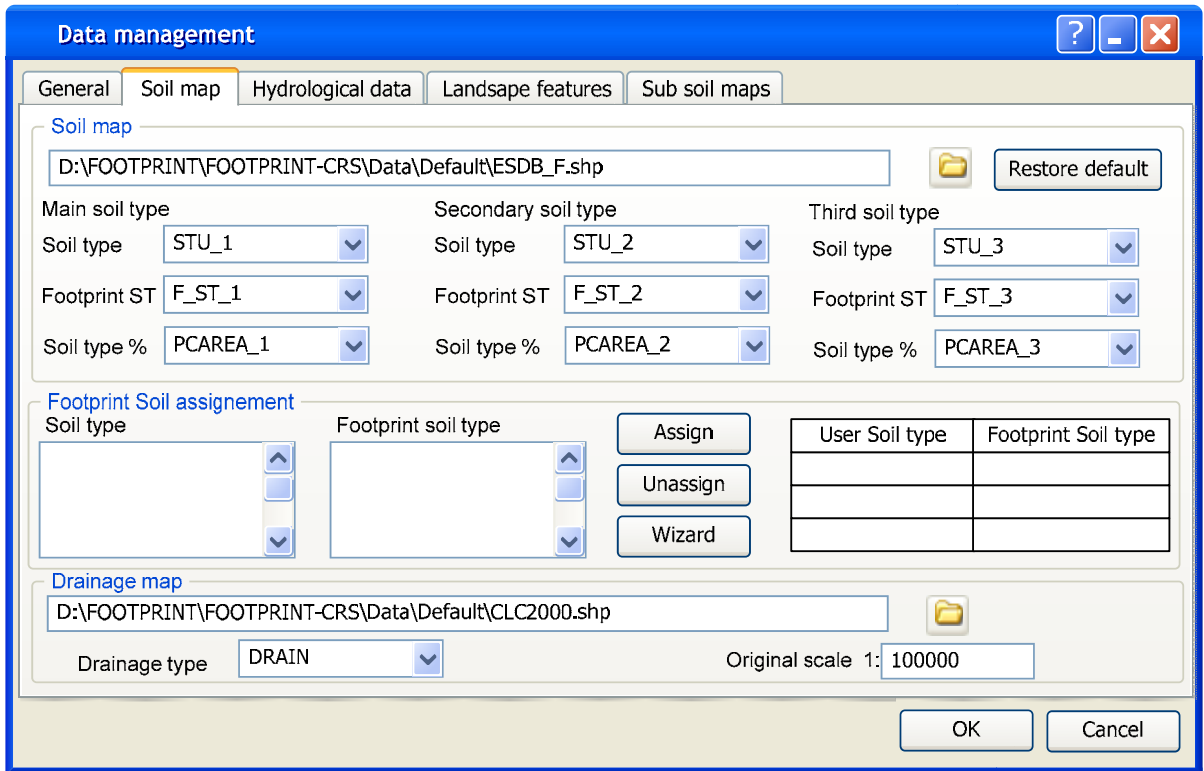


Figure 3b. FOOT-CRS Data management GUI – Soil map

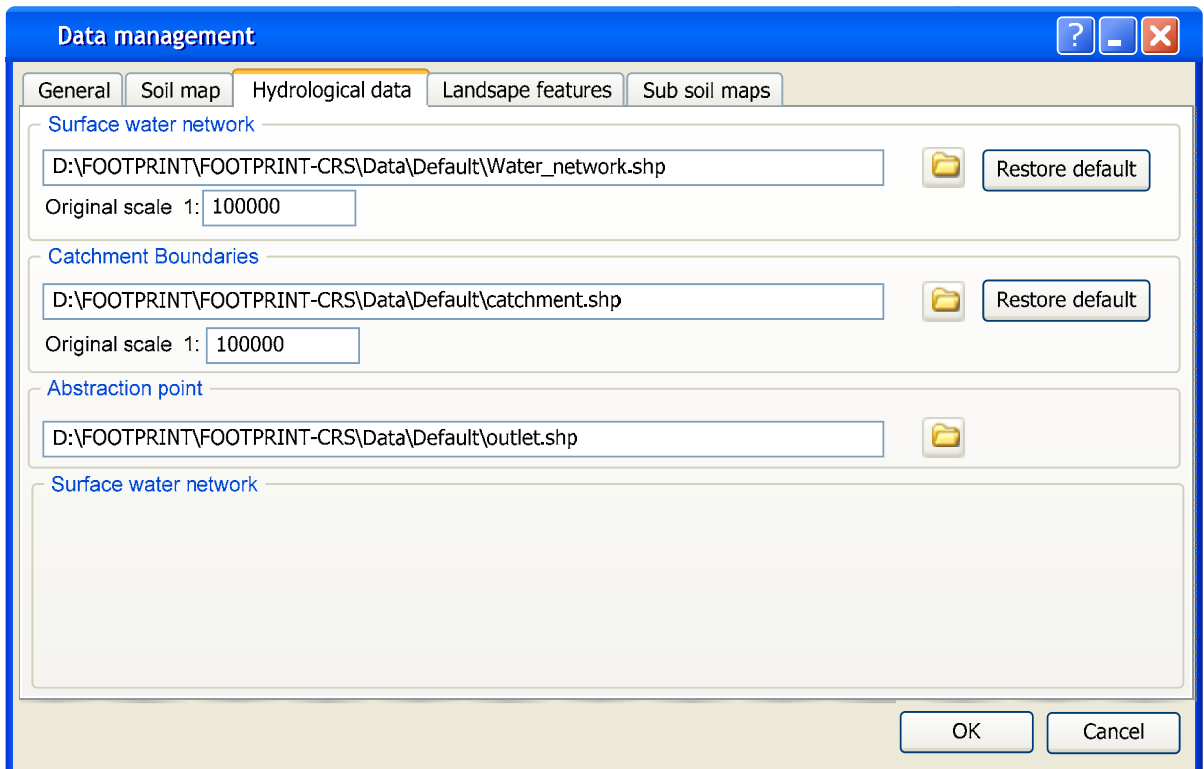


Figure 3c. FOOT-CRS Data management GUI – Hydrological data

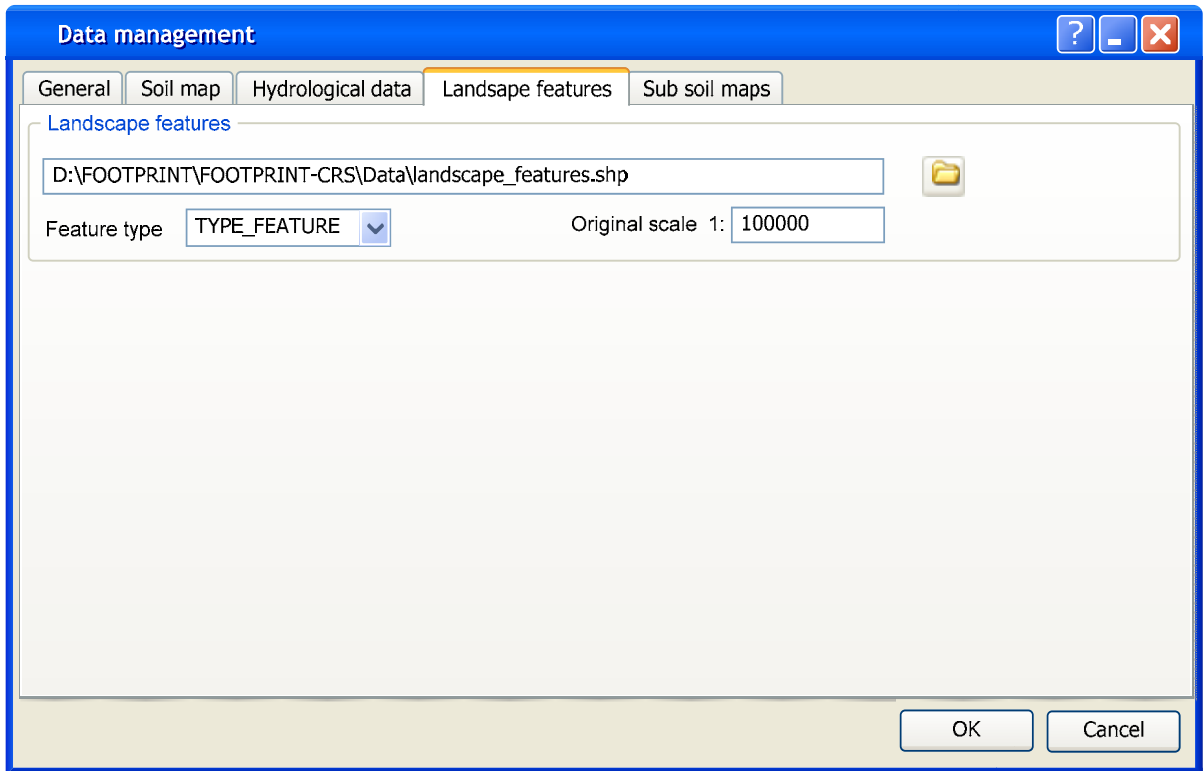


Figure 3d. FOOT-CRS Data management GUI – Landscape features



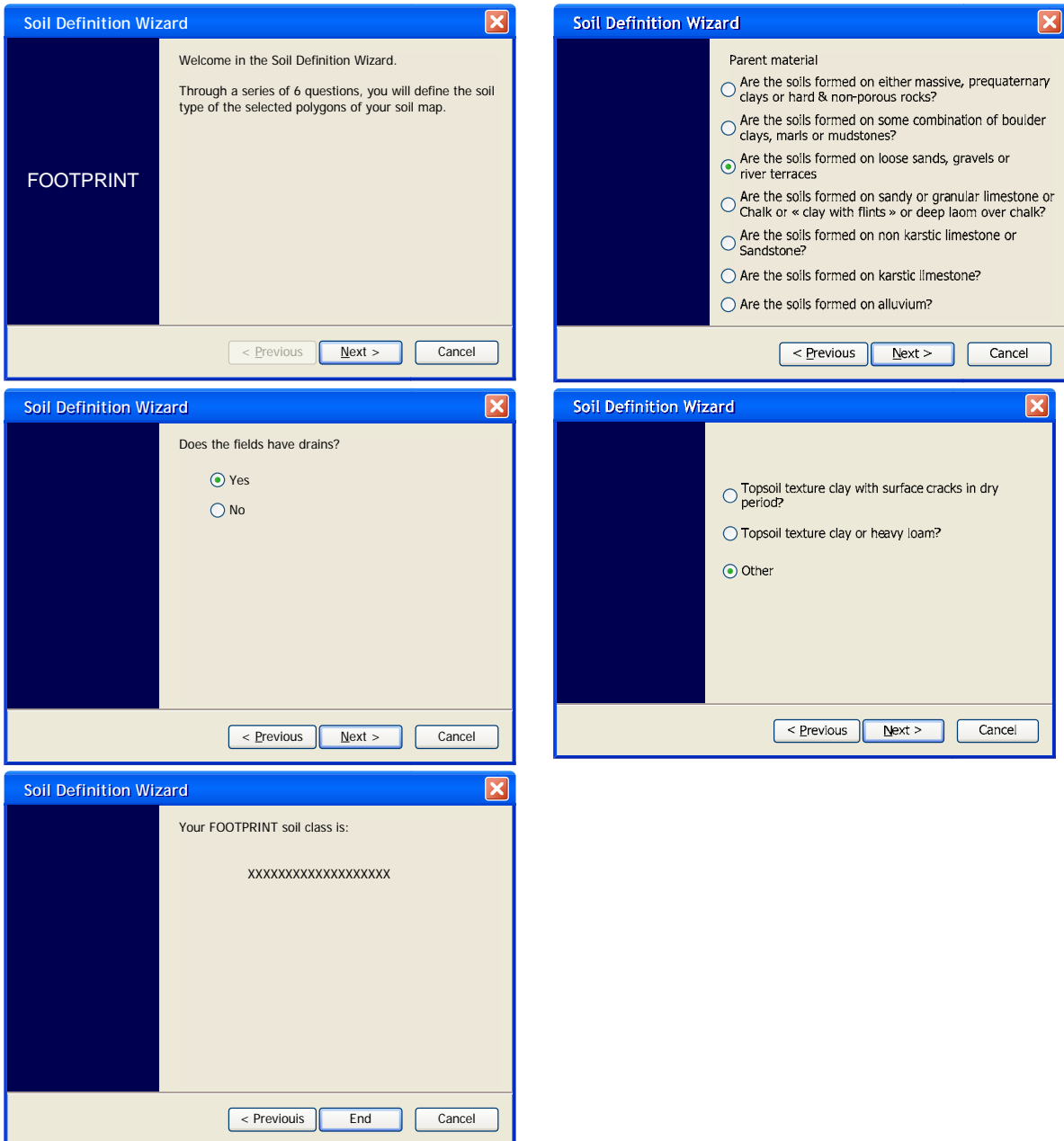


Figure 4. FOOTPRINT soil definition wizard (accessible from the wizard button in the Soil map thumbnail of the Data management window)

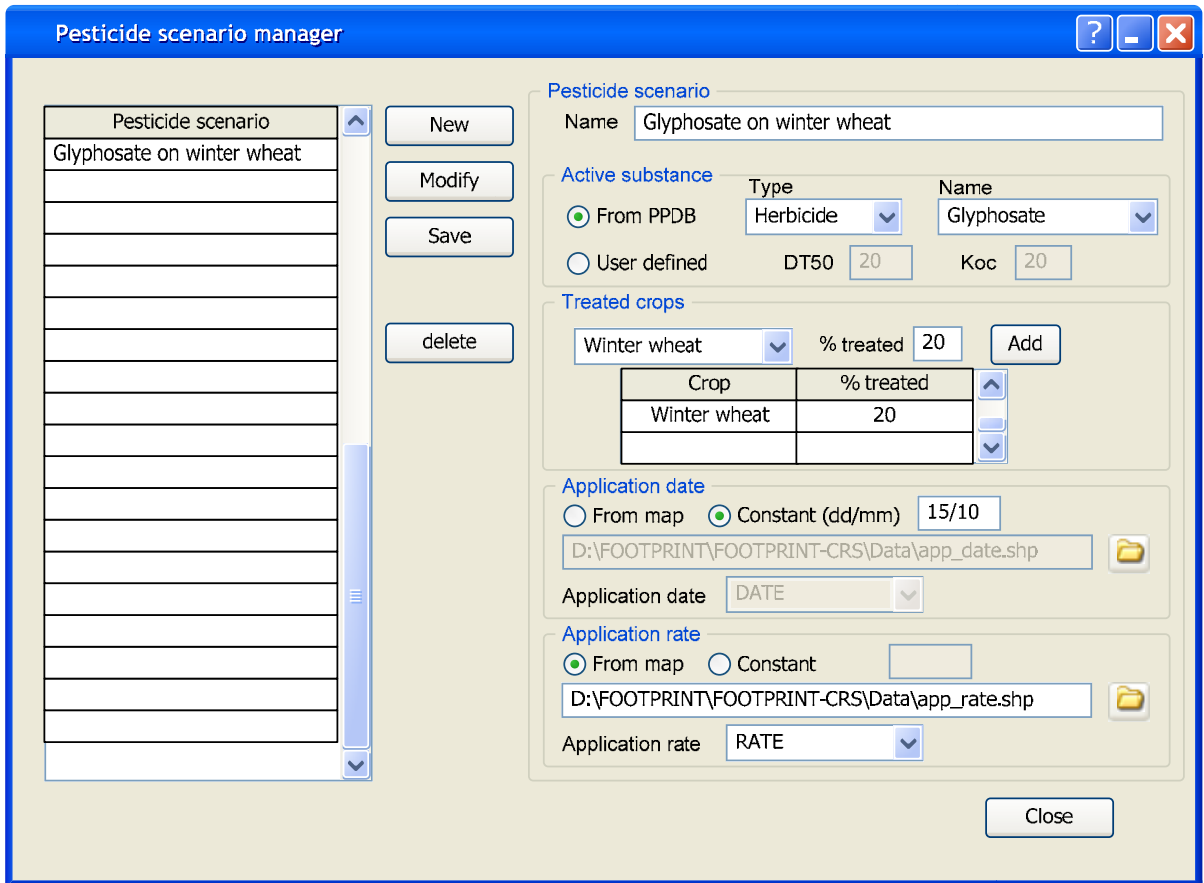


Figure 5. FOOT-CRS Pesticide scenario manager window

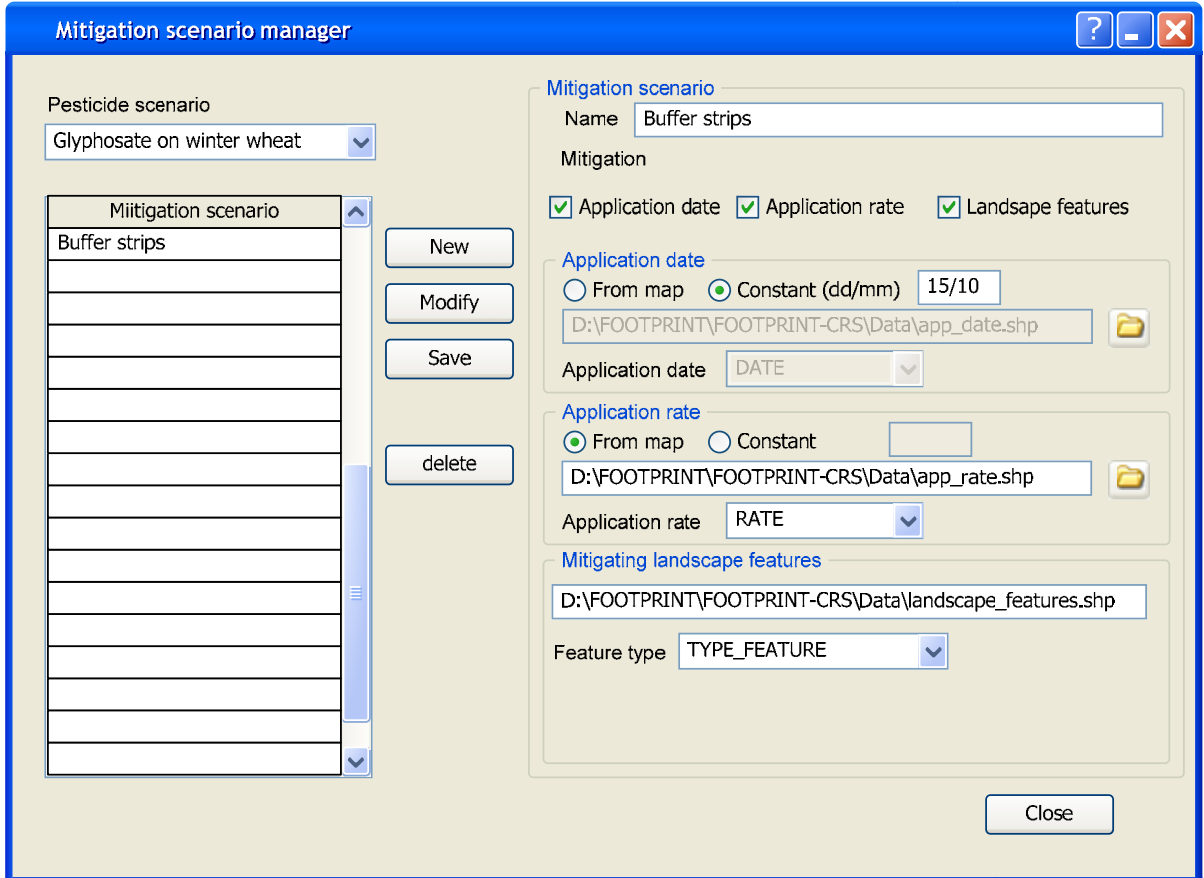


Figure 5. FOOT-CRS Mitigation scenario manager window



## 4.5 Software management

### 4.5.1 Bug fixing and software upgrades post release v.1

A software bug is an error, failure, or fault in a software program that prevents it from behaving as intended. Bugs can arise from errors made during the program coding process and/or during its design. They can have a wide variety of effects, with varying levels of inconvenience to the user of the program. Serious bugs may cause a software program to stop operating i.e. to crash or to freeze. Usually these bugs will be identified during bench and beta testing exercises. However, some bugs may only occur in very specific circumstances or only with particular data sets. These usually have only a subtle effect on the program's functionality and so may lie undetected for a long time. It is virtually impossible to test and evaluate a software program's performance with every possible set of input data or in every possible way an end user may operate it. Consequently, it is rare for a software program to be completely bug-free. Therefore it is important that procedures are put in place for end users to report bugs, for bugs to be fixed and upgrades or software patches distributed.

The FOOTPRINT website will have facilities for users to report bugs directly to the software developers and to provide (wherever possible) the input data causing the problem. This is particularly important as it is not always easy to reproduce bugs. Some bugs are triggered by inputs to the program that may be difficult for the programmer to re-create.

Once the bug has been identified and fixed a corrected version of the module at fault will be available for download from the FOOTPRINT website. Details regarding the error and bug fix will be also logged on the website. Each new release will be given a unique version number for reference.

### 4.5.2 Software upgrades

From time to time it may be necessary for scientific or technical reasons to revise the software and/or the underpinning databases. If and when this occurs a new version of the module or modules revised will be available on the FOOTPRINT website for download. Details of the upgrade, technical changes and release date will also be logged on the website. Each new release will be given a unique version number for reference.

### 4.5.3 Maintenance

Maintenance and updating will be performed by Olivier Francois at GEOSYS during the development phase. After the end of the FOOTPRINT in December 2008 project a maintenance structure has to be established for all 3 tools.

## 5 THE CORE SYSTEM

### 5.1 System Shell

The FOOT-CRS system shell will be integrated in the ArcGIS shell. It will include:

- Menus (integrated in the ArcGIS menu bar) allowing the user to navigate through the modules to complete an exposure assessment. Menu items will be direct links to the relevant modules and tools.
- Buttons to compute new information from existing data (e.g. compute a new map layer)
- Buttons to open a screen or dialogue of a module or tool (alternative path to the menus)
- Help and support including:
  - General introductory text to FOOT-CRS, the other FOOTPRINT tools and the FOOTPRINT project.



- General help text regarding the operation of the FOOT-CRS system and the tools and facilities available.
- Links to the FOOTPRINT website
- Upgrading and updating tools showing module versions numbers, availability of upgrades and automatic upgrade functions.

FOOT-CRS will consist of eight different modules (cf. Tables 1-8). Five of them will have substantial interaction with the user: three modules for data input (Data Management, Pesticide Scenario Manager, Mitigation manager), one for data processing (Landscape analysis), and one for model output (Display + Mapping of Results). The remaining three modules FOOTPRINT Scenario, Dominant Pathways and Modelling are just launched by the user and offer no further interaction.

## 5.2 Data input

For all input data, there are two possibilities for the user depending on data availability:

- Use of the default FOOTPRINT scenarios (FOOTPRINT soil classes, FOOTPRINT agronomic scenarios etc.)
- Input of own data if available at a finer resolution

### 5.2.1 Data Management Module

Soil and land-use spatial data imported by the user in the Data Management module (module 1) are subsequently converted into a map of FOOTPRINT scenarios in the FOOTPRINT scenario module (module 2). To enable this, the user has to assign FOOTPRINT classes to the classes in his own map. To aid the correct assignment of FOOTPRINT soil classes to the soil classes in the user's map, a dedicated wizard is proposed : the user will have to answer basic questions from the Host/Corpen flow chart.

It is proposed to use a Digital Elevation model derived from SRTM data (90 m resolution) as default DEM, and the DEM cells as basic map units. However, the user will be able to import and use a higher-resolved DEM and thus also to have smaller map units.

The data import tools in module 1 must have extensive capabilities:

- adjust variables and classes in attribute tables to the FOOTPRINT data format
- correctly assign FOOTPRINT scenarios to variables and classes in attribute tables of imported maps (assigning has to be done by user, but the implementation of the assignment will be done automatically by the import tools)

The user can also import remote sensing data (satellite imagery; for small catchments also aerial photos) or any other vector data (e.g. topographic maps) for analyzing in the Landscape Analysis module (module 3, cf. section 5.3).

### 5.2.2 Pesticide Scenario Manager

In the Pesticide Scenario Manager (module 5), the user enters all pesticide-related input:

- active ingredient(s) incl. physical and chemical properties (changeable default values provided in the FOOTPRINT PPDB included in FOOT-CRS),
- treated crop(s),
- application rate(s),
- percentage of crop area that is treated
- application date(s).
- The so created pesticide application scenarios can either be applied to the whole area of interest (catchment, region) or only to parts of it.

Also the input necessary for calculation of point source inputs into water bodies will be entered in module 5, e.g. number of farms and field sprayers in the catchment, expected % loss of product by spillage etc.

The module will contain an uncertainty/variability processor for probabilistic risk assessment, to evaluate the effect of variable and/or uncertain parameters in the pesticide scenarios: (compound properties, application rate and date, treated percentage of crop area).

### 5.2.3 Mitigation manager

The Mitigation Manager (module 7) allows the user to define and save different mitigation scenarios. Mitigation measures for reducing pesticide inputs into water bodies can be selected from a predefined list. Changeable default values will be provided for the efficiencies of the various measures. Localized measures such as buffer strips can be entered in a map of user-defined mitigation features, which will be used in the “Conversion of losses to inputs” step (sub-module 6.2) together with the map of mitigation features identified in the landscape analysis.

The module will contain an uncertainty/variability processor for probabilistic risk assessment, to evaluate the effect of variable and/or uncertain properties of mitigation features (density, position, abundance, efficiency).

## 5.3 Pre-modelling phase and meta-modelling

Using spatial data input into the system (cf. Table 1b), the software will i) assign FOOTPRINT scenarios to areas in the catchment (Module 2), ii) identify the dominant pesticide contamination pathways in the landscape (Module 3, cf. Fig. 1), and iii) calculate the trajectories of pesticides transported via surface runoff and drift from each cell to surface water (Module 4). Pesticide property data required to drive the meta-models of MACRO and PRZM (or, for what-if calculations, MACRO and PRZM themselves) will be identified and retrieved from the PPDB (see Section 6.2).

### 5.3.1 Assigning scenarios to areas (FOOTPRINT map units) in the catchment

The situation at the start is:

- A catchment with a gauge or drinking water abstraction site at the outlet.
- „Agro-environmental scenarios” (unique combinations of soil, climate and climate-specific crop scenario), which are somehow distributed over the catchment area.

However, with the Europe-wide default data sets provided by FOOTPRINT the agro-environmental scenarios cannot be localized exactly, because:

- A soil mapping unit (SMU) in the SGDBE has a distribution of soil scenarios (FOOTPRINT soil classes) with different area proportions or probabilities of occurrence each (e.g. 40 % soil A, 20 % soil B etc.).
- A crop mapping unit from CLC2000 has a distribution of crops with different area proportions or probabilities of occurrence each (e.g. 40 % winter wheat, 20 % winter barley, 20 % maize etc.), which are given by the NUTS-2 level agricultural statistics.

That is, each FOOTPRINT map unit has exactly 1 climate scenario, but an area distribution of crops, soils and thus of “agro-environmental scenarios”. As a consequence, scenarios and thus simulated pesticide losses will be assigned to the areas in the catchment statistically, using the following assumptions:

- The areic distribution of FOOTPRINT soil classes is homogeneous over the SMU.
- The areic distribution of crops is homogeneous over the agricultural census unit (which is not realistic of course at NUTS-2 level).

- If there occur unrealistic crop/soil combinations in a FOOTPRINT map unit (e.g. potatoes on a heavy clay), the area of this combination is assumed as zero. The area of the crop is then redistributed proportionally to the other soil classes in the FOOTPRINT map unit.

If the user has own, better resolved soil and/or land use data with only one scenario per soil mapping unit and/or land-use mapping unit, respectively, the assignment of scenarios to FOOTPRINT map units will be considerably easier.

### 5.3.2 Landscape analysis

The main purpose of the Landscape Analysis module (module 3) is to create a map of existing landscape features, including features mitigating pesticide inputs into water bodies (e.g. hedges, buffer strips, grassed waterways).

There are two options for accounting for landscape features mitigating pesticide inputs:

If aerial photos or sufficiently resolved satellite imagery are available, a semi-automatic tool is provided to help the identification of mitigating landscape features. This tool will have capabilities of image processing, (half-) automated object classification, distance calculations etc.

If no aerial photos or sufficiently resolved satellite imagery are available or the catchment is simply too large, the user can choose one or more landscape types from photos provided in FOOT-CRS of reference landscapes with different types and differing density and position of mitigating landscape elements (for drift + runoff/erosion). The locations of these landscape types in the catchment are determined by the user. The presence of mitigating landscape elements in the catchment will then be estimated statistically from the reference landscape types.

### 5.3.3 Calculate map of dominant contamination pathways and trajectories of pesticides to surface water

The Dominant Pathways module (module 4) will have two main functions:

1. Create a map of dominant contamination pathways. This map will state whether an area is more prone to pesticide losses via surface runoff/erosion, drainflow, drift or leaching, and constitutes one of the main FOOT-CRS outputs. The dominant contamination pathways for each map unit will be obtained by decision rules adapted from those used in the FOOT-FS tool for the use at the catchment scale. For larger catchments, also the IDPR methodology will contribute information on dominant pathways. The dominant pathways map will be computed for two seasons (field capacity period and soil moisture deficit period) and be displayed in a colour-coded format. It has to be kept in mind (and will be explicitly communicated to the user) that this information is only qualitative, and that the absolute and relative contributions of the different pathways to pesticide contamination of water resources can vary dramatically from year to year.

2. Calculate trajectories of pesticides from each map unit (= DEM cell) to the nearest surface water body/bodies.

- Surface runoff and erosion: downhill flowpath using DEM + flow length calculation
- Drift: straight lines in 8 directions (N, NE, E, SE, S, SW, W, NW) + distance calculation

### 5.3.4 Modelling and meta-modelling

Mathematical modelling is the process of creating a simplified mathematical representation of a real-world process in order to gain a better understanding of it. It is a process that attempts to match observation with a mathematical description. During the process of building the model, in order to simplify the mathematical representation, the developer must decide what factors are relevant to the problem and what factors can reasonably be ignored. The consideration and incorporation of more factors may well improve the models performance but this is often a trade-off against the models run-time and the computing power required for its operation. For scientists and regulators long model run-times of 1 or more hours with a complex model such as MACRO

may be acceptable, but at the catchment scale, where dozens or hundreds of model runs might be necessary, the required computation time would definitely be too long. Therefore, a meta-model approach is followed in FOOT-CRS. This requires model simulations (MACRO and PRZM) to be run beforehand for all potential combinations of FOOTPRINT agro-environmental scenarios and pesticide property data (normalized sorption coefficient  $K_{oc}$  and soil dissipation half-life DT50).

From the MACRO and PRZM simulations, 20-year daily time series for water fluxes and pesticide losses will be available for:

- Leaching at 1 m depth (MACRO)
- Drainage (MACRO)
- Infiltration excess runoff (PRZM)
- Saturation excess runoff (MACRO or PRZM)
- Subsurface flow (MACRO)

Since the time series themselves cannot be distributed with the software due to storage issues, meaningful summary statistics must be derived and provided with the tools. Which summary statistics (min, max, median, mean, a number of percentiles etc.) have to be stored and distributed with the software depends on the PEC calculation methods and on user needs. It is furthermore being discussed whether various pesticide loss percentiles for the whole time series are sufficient or loss percentiles for each calendar month are needed.

The selected results from the meta-modelling exercises will then be formatted into look-up tables and stored as a suite of MS Access database files. Data from these will be retrieved based on the  $K_{oc}$  and DT50 of the pesticide being modelled. The pesticide  $K_{oc}$  and DT50 will be retrieved directly from the FOOTPRINT PPDB (see Section 6.1) although facilities will be incorporated to override this default with the users own data.

## 5.4 Exposure assessment

Using the results from the meta-modelling and landscape analysis activities, the predicted environmental concentrations (PEC) in edge-of-field surface water bodies, surface water abstraction points at the catchment outlet and groundwater will be calculated (Module (6)). Concentrations will be estimated considering potential dilution effects based on the size and discharge of the water body, water volumes associated with runoff and drainage inputs and the presence of bed sediment.

The main outputs will be annual average leachate concentrations in 1 m depth (“PEC<sub>gw</sub>”), and PEC<sub>sw</sub> distributions at the catchment outlet separately for each input pathway.

Since the main focus at the catchment scale is water quality for human consumption (and thus, the drinking water limit of 0.1  $\mu\text{g L}^{-1}$ ), no TER calculations will be performed in FOOT-CRS. However, the exposure distributions provided to the user will enable him to do so if he likes. A tentative methodology for exposure assessment in FOOT-CRS is given in the following.

### 5.4.1 Surface water exposure assessment for the catchment outlet

Calculation of Predicted Environmental Concentrations in surface water (PEC<sub>sw</sub>) and risk assessment are relatively straightforward in FOOT-FS und FOOT-NES, since only „edge-of-field“ water bodies are considered. At the catchment scale the aim is concentrations at the outlet, however, or even Exceedance frequencies of  $x \mu\text{g L}^{-1}$  (usually 0.1  $\mu\text{g L}^{-1}$ ) in a given period. This implies that results must be aggregated meaningfully. It must be taken account of the following phenomena:

- different flow lengths and travel times from each field to the catchment outlet („geomorphological dispersion“)
- transport and dispersion in the water course
- sorption and degradation in the water course

- spatial and temporal variability of weather and application dates

It is proposed to estimate loads and PEC<sub>sw</sub> at the catchment outlet separately for each input path. For instance, surface runoff might lead to higher peak concentrations at the outlet, but to less frequent exceedances of 0.1 µg L<sup>-1</sup> than drift inputs. Having the PEC separately for each pathway will also make it easier to recommend mitigation measures and evaluate their effect at the catchment scale. This method can be justified because the input events from the different pathways probably will not coincide on the same date.

Currently proposed general method for exposure assessment at the catchment outlet (for each input path separately):

- calculate pesticide (and water volume and eroded sediment, where applicable) losses from each pixel, separately for each agro-environmental scenario occurring in this pixel
- select a given percentile (e.g. the 99.7<sup>th</sup>) of the pesticide loss for each pixel, separately for each agro-environmental scenario in this pixel, and the corresponding surface runoff volume + eroded sediment or drainage volume
- convert losses to inputs into surface water
- Drift and Runoff/Erosion: For each pixel the pathway of pesticides to the nearest water body is traced in the GIS (module 4). Using the resulting map of trajectories, the shares of pesticide losses from each pixel that eventually reach a water body are calculated, taking account for mitigation landscape elements on the trajectories. Detailed methodology is still to be finalised.
- Drainage: We assume that everything that enters the drains will reach the surface water bodies.
- Point sources: Methodology still to be worked out.
- sum up these inputs over the catchment → X<sup>th</sup> (99.7<sup>th</sup>) percentile load for the whole catchment.
- Divide by the sum of the daily discharge at the catchment outlet and the surface runoff and drainflow contribution from the catchment pixels. Monthly mean river discharges can be obtained freely on a half-degree basis for the whole of Europe from the GRDC in Koblenz; also daily discharge series of single stations are available. The result of this calculation is a fictitious “initial” X<sup>th</sup> (99.7<sup>th</sup>) percentile concentration
- apply an equation analogous to the Convection-Dispersion Equation CDE (e.g. Gustafson’s equation (Gustafson et al., 2004, supporting information) or a modification of it) to this fictitious „initial“ concentration, using the mean river length in the catchment (computed from surface water network) and a generic mean streamflow velocity. The result is a “X<sup>th</sup> (99.7<sup>th</sup>) percentile” PEC<sub>sw</sub> at the outlet (though admittedly uncertain).
- Repeat steps 2.-6. for other percentiles of the input time series.
- Read off the frequency / return period for each percentile → interpolate frequency of exceedance of e.g. 0.1 µg L<sup>-1</sup>

#### 5.4.2 Mathematical description of exposure calculations for surface water

##### Drainage inputs

$$L_{sw,drain\_X} = \sum_r \sum_c \sum_s \{ X^{th-\delta} MACRO(STC, Climate, CropScen, AppDate) \times relDoser_{,c} \times AA\%_r \times Crop\%_{r,c} \times CropTreat\%_{r,c} \times STC\%_{r,s} \times AAdrain\%_r \times MFdrain\%_r \times UnitArea_r \}$$

Where

$L_{sw,drain\_X}$  = X<sup>th</sup> percentile daily input of a.i. into surface waters via tile drains in the area of interest [mg]

$X^{th-\delta} MACRO(STC, Climate, CropScen, AppDate)$  = X<sup>th</sup>-percentile of the 20-year MACRO meta-model simulation results on tile drainage loss (% of dosage) of a.i. as a function of soil type class, climate, crop growth and date of application [mg/ha]





|                                    |  |
|------------------------------------|--|
| relDoser <sub>r,c</sub>            | = application rate of a.i. to crop c in map unit r, relative to the standard rate of 1 kg ha <sup>-1</sup> of the MACRO meta-model simulation [%]                        |
| AA% <sub>r</sub>                   | = Percentage of arable land, permanent cultures etc. in map unit r [%]   |
| Crop% <sub>r,c</sub>               | = Percentage of AA in map unit r cropped with field crop c [%]   |
| CropTreat% <sub>r,c</sub>          | = Percentage of crop c treated with the a.i. (reflects plant protection intensity and “market share”) [%]  |
| STC% <sub>r,s</sub>                | = Percentage of soil type class s in the Soil Mapping Unit [%]   |
| AA <sub>drain</sub> % <sub>r</sub> | = Percentage of AA with tile drainage in map unit r [%]  |
| M <sub>Fdrain</sub> % <sub>r</sub> | = Mitigation factor, reflecting the effects of reduction measures for tile drainage inputs from map unit r [%]   |
| UnitArea <sub>r</sub>              | = Area of the map unit r [ha]  |
| r                                  | = Map unit index   |
| c                                  | = Crop index (if a summation over different crops is intended, it will be necessary to calculate the loss percentiles of the MACRO/PRZM time series on a monthly basis). |
| s                                  | = Soil class index   |

### Surface runoff and erosion inputs

$$L_{sw,runoff\_X} = \sum_r \sum_c \sum_s \{X^{th-\delta PRZM}(STC, Climate, CropScen, AppDate) \times relDoser_{r,c} \times AA\%_r \times Crop\%_{r,c} \times CropTreat\%_{r,c} \times STC\%_{r,s} \times ConF\%_r \times M_{Frunoff}\%_r \times UnitArea_r \}$$

where

|   |   |
|---|---|
| L <sub>sw,runoff_X</sub>                                | = X <sup>th</sup> percentile daily input of a.i. into surface waters via surface run-off and soil erosion in the area of interest [mg]  |
| X <sup>th</sup> -δPRZM(STC, Climate, CropScen, AppDate) | = X <sup>th</sup> -percentile of the 20-year PRZM simulation results on runoff loss (% of dosage) of a.i. as a function of soil type class, climate, crop growth and date of application [mg/ha]                                    |
| relDoser <sub>r,c</sub>                                 | = application rate of a.i. to crop c in map unit r, relative to the standard rate of 1 kg ha <sup>-1</sup> of the PRZM simulation   |
| AA% <sub>r</sub>  | = Percentage of arable land, permanent cultures etc. In map unit r [%]  |
| Crop% <sub>r,c</sub>                                    | = Percentage of AA in map unit r cropped with field crop c [%]  |
| CropTreat% <sub>r,c</sub>                               | = Percentage of crop c treated with the a.i. (reflects plant protection intensity and “market share”) [%]   |
| STC% <sub>r,s</sub>                                     | = Percentage of soil type class s in the Soil Mapping Unit [%]  |
| ConF% <sub>r</sub>                                      | = Connection factor, expressing the degree of connectivity for run off and erosion input from treated fields into surface waters in map unit r [%]  |
| M <sub>Frunoff</sub> % <sub>r</sub>                     | = Mitigation factor, reflecting the effects of reduction measures for pesticide run-off & erosion inputs from map unit r [%] (The two factors ConF% <sub>r</sub> and M <sub>Frunoff</sub> % <sub>r</sub> can possibly be combined.) |
| UnitArea <sub>r</sub>                                   | = Area of the map unit r [ha]   |
| r   | = Map unit index  |
| c   | = Crop index  |
| s   | = Soil class index  |

The approach for erosion will be analogous to the one for surface runoff and is hence not listed here explicitly.

### Spray drift inputs

For 8 possible wind directions (N, NE, E, SE, S, SW, W, NW), the drift input into surface water bodies in the catchment is calculated with the following formula:

$$L_{sw,drift,dir\_X} = \sum_r \sum_c \{ X^{th}\text{-drift\_loading}(\text{Sprayer, Distance in Wind Direction, Season}) \times \text{absDoser}_{r,c} \times AA\%_r \times \text{Crop}\%_{r,c} \times \text{CropTreat}\%_{r,c} \times \text{CropAdj}\%_{r,c} \times SWD_r \times MF_{drift}_r \times \text{UnitArea}_r \}$$

where

$L_{sw,drift,dir\_X}$  =  $X^{th}$  percentile daily input of an a.i. into surface waters via spray drift in the area of interest, for a given wind direction [mg]

$X^{th}\text{-drift\_loading}(\text{SprayerType, Distance, Season, River Width})$  = estimated  $X^{th}$ -percentile drift loading values as a function of sprayer type (boom vs. air blast sprayer, +/- drift reducing equipment), distance edge-of-field to adjacent water body, crop stage at application (early vs. late season, only for air blast applications), and river width [% (1. It must also be possible to specify legal minimum spraying distances. 2. The choice of the percentile must be discussed. Leave choice to user? On the catchment scale, the 50<sup>th</sup> percentile might be more relevant in some cases.)

$\text{actDoser}_{r,c}$  = Application rate (actual) of a.i. to crop c in map unit r [kg/ha]

$AA\%_r$  = Percentage of arable land, permanent cultures etc. in map unit r [%]

$\text{Crop}\%_{r,c}$  = Percentage of AA in map unit r cropped with field crop c [%]

$\text{CropTreat}\%_{r,c}$  = Percentage of crop c treated with the a.i. (reflects plant protection intensity and “market share”) [%]

$\text{CropAdj}\%_{r,c}$  = Percentage of fields with crop c adjacent to surface waters within a critical distance relevant for spray drift input in map unit r [%](If we can perform a routing from every pixel to the nearest water body, this factor is unnecessary)

$SWD_r$  = Density of surface water network in map unit r [km/km<sup>2</sup>] (If we can perform a routing from every pixel to the nearest water body, this factor is unnecessary)

$MF_{drift}_r$  = Mitigation factor, reflecting the effects of reduction measures for spray drift inputs from map unit r [%]

$\text{UnitArea}_r$  = Area of the map unit r [ha]

r = Map unit index, summed up over area of interest

c = Crop index

The variable  $X^{th}\text{-drift\_loading}$  will be calculated using the drift equation proposed by FOCUS (2001). The different percentiles will be obtained by fitting the parameters of the FOCUS drift equation to the different percentiles of the BBA drift tables (Rautmann, 2001) or of the raw data of the BBA drift trials.

The drift inputs into the catchment for the different wind directions will be averaged using the unweighted or a weighted (with the probabilities of occurrence of the different wind directions) arithmetic mean. The weighting has to be done by the user.

### Point source inputs

Assessment methodology as well as necessary user inputs are still being discussed. The model HARDSPEC (Hollis et al., 2004) is most probably too complex and requires too many input data. A simpler approach like the one from Garratt and Kennedy (2006) is being sought.

### PEC<sub>sw</sub> at the catchment outlet

No summation over input pathways is performed here, since a coincidence of peak concentrations from the different input pathways on the same day is unrealistic. PEC<sub>sw</sub> for each pathway are therefore assessed separately.

$$PEC_{sw,drain\_X} = L_{sw,drain\_X} / (Q(t) + D(t)) \times GF$$

$$PEC_{sw,runoff/erosion\_X} = (L_{sw,runoff\_X} + L_{sw,erosion\_X} \times ERF) / (Q(t) + R(t)) \times GF$$

$$PEC_{sw,drift\_X} = L_{sw,drift\_X} / Q(t) \times AF \times GF$$

where

- $PEC_{sw,drain\_X}$  =  $X^{th}$  percentile daily  $PEC_{sw}$  at the catchment outlet resulting from drainage inputs [ $mg\ m^{-3} = \mu g\ L^{-1}$ ]
- $PEC_{sw,runoff/erosion\_X}$  =  $X^{th}$  percentile daily  $PEC_{sw}$  at the catchment outlet resulting from surface runoff and erosion inputs [ $mg\ m^{-3}$ ]
- $PEC_{sw,drift\_X}$  =  $X^{th}$  percentile daily  $PEC_{sw}$  at the catchment outlet resulting from spray drift inputs [ $mg\ m^{-3}$ ]
- $L_{sw,drift\_X}$  =  $X^{th}$  percentile daily input of an a.i. into surface waters via spray drift in the area of interest, averaged over the 8 different wind directions [mg]
- $Q(t)$  = daily river discharge from area of interest [ $m^3$ ] (either available as monthly means or as Flow Duration Curves)
- $R(t)$  = daily surface runoff volume from area of interest [ $m^3$ ], corresponding to  $L_{sw,runoff\_X}$
- $D(t)$  = daily drainflow volume from area of interest [ $m^3$ ], corresponding to  $L_{sw,drain\_X}$
- $GF$  = Peak Concentration Reduction Factor from Gustafson equation (or another CDE analogon). The Gustafson equation converts a pulse input into a breakthrough curve at the catchment outlet → the peak concentration at the outlet will be lower than “input / discharge”.
- $ERF$  = Reduction factor for contribution of pesticide inputs adsorbed to eroded sediment to pesticide concentrations in the water phase ( $PEC_{sw}$ ). It must be accounted for here that not all adsorbed pesticide will contribute to  $PEC_{sw}$  (strongly sorbing pesticides will remain adsorbed to particles to a large extent).
- $AF$  = Application factor. Equals the maximum proportion of the treated crop area in the catchment that is sprayed on the same day. This reduction factor is necessary because the larger the catchment is, the more unlikely it is that all treated fields in the catchment are sprayed on the same day. The application factor must be specified by the user, bearing in mind the size of the catchment and the number of farmers and sprayer operators in the catchment.

### Mathematical description of exposure calculations for groundwater

$$PEC_{gw,1m\_X,r} = \sum_c \sum_s \{ \delta MACRO(STC, Climate, CropScen, AppDate) \times relDoser_{,c} \times AA\%_r \times Crop\%_{r,s} \times CropTreat\%_{r,c} \times STC\%_{r,s} \times MFleach\%_r \}$$

where

- $PEC_{gw,1m\_X,r}$  =  $X^{th}$  percentile annual flux concentration of a.i. in the leachate in 1 m depth [ $\mu g\ L^{-1}$ ] in map unit r
- $\delta MACRO(STC, Climate, CropScen, AppDate)$  =  $X^{th}$  percentile of annual average flux concentration from the 20-year MACRO simulation results (1 m depth) of an a.i. as a function of soil type class, climate, crop growth and date of application [ $\mu g\ L^{-1}$ ]
- $relDoser_{,c}$  = application rate of a.i. to crop c in map unit r, relative to the standard rate of  $1\ kg\ ha^{-1}$  of the MACRO simulation [%]
- $AA\%_r$  = Percentage of arable land, permanent cultures etc. in map unit r [%]
- $Crop\%_{r,c}$  = Percentage of AA in map unit r cropped with field crop c [%]
- $CropTreat\%_{r,c}$  = Percentage of crop c treated with the a.i. (reflects plant protection intensity and “market share”) [%]
- $STC\%_{r,s}$  = Percentage of soil type class s in the Soil Mapping Unit
- $MFleach\%_r$  = Mitigation factor, reflecting the effects of reduction measures for leaching losses from map unit r [%]
- r = Map unit index

- c = Crop index
- s = Soil class index

For leaching, the PEC calculation methods are the same in FOOT-CRS and FOOT-NES. Pesticide concentrations in depths greater than 1 m will be assessed only qualitatively (cf. FOOTPRINT Deliverable DL10 (Højberg et al., 2006)).

*Database holding necessary information for exposure calculations*

| Variable  | Content, Source  | Availability   |
|---|--|--|
|   |  |  |
| δPRZM(STC, Climate, CropScen, AppDate)            |  | FOOTPRINT simulation runs  |
| δMACRO(STC, Climate, CropScen, AppDate)           |  | FOOTPRINT simulation runs  |
| STC   | Soil Type Class No., Map of Soil Mapping Units (SMU) 1:1M from SGDBE (ca. 100...150 STU), a SMU has different STC (percentages given)                        | FOOTPRINT soil scenarios   |
| Climate   | Climate scenario no. (20-y weather time series); map of European Climatic zones (ca. 15 zones)   | FOOTPRINT climate scenarios  |
| CropScen  | Crop growth stage scenario no. (ca. 25)  | FOOTPRINT agronomic scenarios                                      |
| AppDate   | Date of application (12 or 24 dates available for selection)   | user input   |
| Xth-drift_loading (SprayerType, Distance, Season) |  | FOCUS (2001), BBA drift tables / raw data                          |
| SprayerType                                       | Type of sprayer, depends on crop type  | determined by crop, may be overridden by user in some cases        |
| Distance  | distance between treated field and surface water body  | calculations in GIS  |
| Season  | Application season, depends on AppDate   | ---  |
| actDoser <sub>c</sub>                             | Actual application rate  | user input   |
| AA% <sub>r</sub>                                  | CORINE 2000 map (classes 211, 212, etc.); possibly needs scaling with agricultural census data due to generalization error and minimum size of mapping units | One map for EU25   |
| Crop% <sub>r,c</sub>                              | Tables: Agricultural Census on NUTS-2 level<br>Shape of NUTS-2 polygons  | EUROSTAT?  |
| CropTreat% <sub>r,c</sub>                         | Percentage of crop c treated with the a.i. (reflects both the plant protection intensity in that crop and catchment and the “market share”)                  | user input   |
| ConF% <sub>r</sub>                                | Connectivity factor  | Can maybe be combined with MFrunoff                                |
| CropAdj% <sub>r,c</sub>                           | Percentage of treated fields adjacent to a surface water body, map   | probably not necessary   |
| SWD <sub>r</sub>                                  | Density of the surface water network, map  | probably not necessary; can be computed from surface water network |
| MFdrain% <sub>r</sub>                             | Effect of mitigation measures on tile drainage (relevant?)   | user input; probably not relevant                                  |
| MFrunoff% <sub>r</sub>                            | Effect of mitigation measures on run-off   | user input; changeable default (adapted from mitigation review)    |
| MFdrift% <sub>r</sub>                             | Effect of mitigation measures on spray drift   | user input, changeable default (adapted from mitigation review)    |
| MFleach% <sub>r</sub>                             | Effect of mitigation measures on leaching (relevant?)  | user input; probably not relevant                                  |

|                       |   |                          |
|-----------------------|---|--------------------------|
| UnitArea <sub>r</sub> | Area of a mapping unit (grid cell, cone sector), map        | to be constructed        |
| Not named             | River basins, catchments, map                               | CCM 2                    |
| Not named             | Other shapes with areas of interest, map                    | ??                       |
| Slope                 | derived from modified SRTM elevation data (resolution 90 m) | From DTM                 |
| Q(t)                  | monthly mean discharge (MMQ) or Flow Duration Curves (FDC)  | GRDC in Koblenz, Germany |

## 5.5 Communication and reporting of results

Communication, reporting and mapping of results will be performed in Module 8. Within this module, a suite of decision rules will be used to interpret the calculated exposure distributions and identify appropriate mitigation and management activities. The module will facilitate to

- Display maps of dominant contamination pathways
- Display PEC maps (for each pathway), and change legend
- Display figures (+explanatory text) from the modelling (e.g. CDF)
- Display summary text (report).
- Display proposed mitigation strategies
- Export maps and reports in different formats.

Due to the large uncertainties at the catchment scale, the presentation of colour-coded schemes is preferable to the presentation of sharp numbers. All presented results will be accompanied by a qualitative or quantitative estimate of uncertainty.

The recommendations of mitigation strategies will also include considerations how these mitigation strategies may influence contamination by other pollutants such as phosphate or nitrate. It is important to pursue integrated approaches to water management rather than merely shifting the problem from one pollutant class to another.

## 6 ADDITIONAL FACILITIES

### 6.1 Pesticide Properties Database

The performance and reliability of mathematical models is ultimately governed by the quality of the model input data. Whilst there are a wide range of sources for the type of input data that will be required by FOOT-CRS not all are of the highest quality and a certain amount of experience and understanding of the science driving the model is required to choose the best data available. The FOOTPRINT PPDB seeks to solve this problem by bring the best sources together in a standardised electronic format. This database will be embedded into the FOOT-FS, FOOT-CRS and FOOT-NES software packages in MS Access 2003 format with Access 2000 file structure to ensure compatibility with most potential users. The database will also be available online.

This database (FOOTPRINT PPDB) will be a comprehensive database of physicochemical and ecotoxicological data relating to pesticide active substances. As the pesticide fate models and meta-models within the FOOT-tools will use the data in the database it is important that the data are of the highest quality possible. The best sources of information currently available are the monographs produced as part of the EU 91/414/EEC review process. These documents will be the first choice for data but they are not available for all pesticides and so alternative sources of data will be used including national government resources, manufacturers, online databases and peer reviewed scientific publications.

Data sets will be cross-checked against each other as a means of ensuring data integrity. Where different sources of data have widely different values these will be validated by comparison with the original publications wherever possible. The database will be actively updated as additional information is identified and new and/or better data becomes available. Each data item will be



'tagged' with a code indicating the confidence the developers have in its quality. Confidence values will be in the range 5 (high) to 0 (low). A low value will not necessarily indicate that the data is incorrect but only that it can not or has not been validated. Confidence values will be based upon:

- The source of the data (e.g. EU dossier, manufacturer, other database or publication). Some existing data sets are no longer being maintained and updated. For example EU dossier data will acquire a confidence value of 5 where as estimated data may acquire a 0 or 1.
- The publication date of the data if known. Very old data may not have been determined using the same scientific procedures, standards and protocols used by the most recent investigations.
- Whether or not the data reference can be identified and used to cross check the data
- The match the data is to the desired parameter. For example the acute toxicity endpoint for fish required is the 96hr LC50 for Rainbow trout (*Oncorhynchus mykiss*) or Bluegill sunfish (*Lepomis macrochirus*). If an exact match can not be identified but data for a different species or a longer duration is available this will be used but the confidence score amended appropriately.
- A judgement on the fitness for purpose will also be made. For example dissipation data for European soils are preferred to those where conditions and soil types are very different.

The database will hold:

- General data describing the chemical such as its appearance, chemical structure and formula and in which EU States it is registered for use.
- Environmental fate data. For example the pesticide octanol-water partition coefficient (Log P), normalized sorption coefficient (Koc) and soil dissipation half-life (DT50).
- Ecotoxicological data. For example acute and chronic endpoint data for fish, aquatic invertebrates and aquatic plants.

## 6.2 Multi-lingual translations

As introduced in Section 3.2 the FOOT-CRS software will be tri-lingual. This will be achieved using software development tools that handle the translation automatically at software run-time. However, to achieve this an electronic language dictionary is required. All strings used in the user-interface (including pesticide active substance common names) will be held in a MS Access database and referenced by an Identification Number (IN).

Against each Identification Number in the database the translations are held for each language. In the software development phase the Identification Number is held rather than the string itself. At run-time the Identification Number is automatically replaced by the appropriate string in the chosen language.

The following language translations are planned: English, French and German. The integrity of the translations is being addressed by ensuring that the translation is carried out by the appropriate FOOTPRINT partner i.e. a native language speaker also fluent in English. The responsible persons for the integrity of the language translations are Kathy Lewis (English), Olivier François (French) and Stefan Reichenberger (German).

## 6.3 User help and support facilities

User support facilities will be embedded into the FOOT-CRS software at all operational levels. The types of help that will be available will include:

- Standard indexed help text and glossaries. This will comprise of written descriptions of both the operational and technical aspects of FOOT-CRS.
- The User Manual in an electronic format will be available for browsing.
- Screen by screen support providing guidance on data entry and data requirements.



Help and support will be accessible to users via a variety of methods including:

- A separate FOOT-CRS help menu in the ArcGIS menu bar
- All FOOT-CRS data input and output screens will have Help buttons and Help icons. Help buttons will link users directly with specific Help text, bypassing the Help index. Help icons will be used to provide additional support such as explaining data input needs at a particular part of the software.
- Each part of the GUI's architecture (i.e. menus, data input boxes, buttons etc) will have associated 'tool-tips'. Tool-tips are used in conjunction with a cursor, usually a mouse pointer. The user hovers the cursor over an item, without clicking it, and a small box appears with the name or description of the item being hovered over.

## **7 EVALUATION, REFINING AND POLISHING PROCESSES**

### **7.1 Evaluation**

The reliability and usability of the FOOT-CRS tool will be assessed through a substantial programme of bench and beta testing, and of evaluation studies for a number of test catchments representing a wide range of agro-environmental conditions in the EU.

Once the first draft of the software is completed a series of in-house bench testing exercises will identify and correct stability problems, obvious bugs and usability short-comings. The bench testing will, among other things, include:

- testing of FOOT-CRS outputs against the standalone MACRO and PRZM meta-models,
- testing of drift calculation algorithms against the standalone equations to ensure that the implementation was error-free.
- testing of shell and database functionality
- testing of correct integration into ArcGIS

On completion of the bench testing a beta-version of the software will be available for testing by FOOTPRINT partners, AC members and any other interested persons.

The beta and final version of FOOT-CRS will benefit from a substantial evaluation exercise where the predictive capability of the tool will be tested using 8 test catchments in Denmark, France, Italy, Poland, Slovenia, Sweden and Switzerland. The exercise will combine on-site evaluation as well as comparisons between tool predictions and monitoring data and/or alternative risk assessment methodologies.

### **7.2 Refinement and software polishing**

Feed-back from the evaluation tests (section 7.1) will provide information on bugs, usability problems, system failures and possible problems with the representation of processes at the catchment scale. These will be corrected and the system refined. If performance bottlenecks (cf. section 7.3) are identified, the code will be refined accordingly to increase resource efficiency of the software.

### **7.3 System performance**

Software performance testing can serve different purposes. It can demonstrate that the system meets performance and/or functionality criteria. It can compare two systems to find which performs or functions better. Or it can measure what parts of the system may cause the system to perform badly or fail. The earlier a performance defect is identified, the easier it is to correct. In all cases, it is often crucial for the test conditions to be similar to the expected actual end use.

Performance testing for FOOT-FS will be undertaken via in-house bench-testing and seek to achieve the following objectives:

- Verify input data collation time. Bench testing will identify typical data input times for users to verify that this is acceptable and to provide user guidance.
- Verify the system capacity versus model run-time. For example, the system could theoretically be used to assess multiple applications of a given pesticide on a number of crops in a diverse catchment with a large number of agro-environmental scenarios. Performance testing will identify when the model run-time becomes unacceptable to end-users or when the data required or generated exceeds software or hardware capacity.
- Determine the optimal hardware/software configuration for FOOT-CRS.

## 8 DOCUMENT MANAGEMENT

This document will be updated as soon it becomes necessary in the development process. Each new document version will supersede its precursor and be labelled with a version number and the date of creation (Table 9).

| <b>Date</b> | <b>Version</b> | <b>Description</b>                                       | <b>Authors</b>                      |
|-------------|----------------|--|-------------------------------------|
| 20/12/2006  | 1.0            | First draft of FOOT-CRS software specification document  | S Reichenberger, O François, M Bach |
| 11/01/2007  | 1.1            | Second draft of FOOT-CRS software specification document | S Reichenberger, O François, M Bach |
|             |                |  |                                     |
|             |                |  |                                     |

**Table 9: Revision history of this document**



## 9 GLOSSARY

### 9.1 Abbreviations, acronyms and proper names

| Abbreviation etc. | Description  |
|-------------------|--|
| CCM2              | Catchment Characterisation and Modelling Database v. 2   |
| CDE               | Convection-Dispersion Equation   |
| CDF               | Cumulative Distribution Function   |
| CLC2000           | CORINE Land Cover 2000   |
| CORINE            | Coordination of Information on the Environment   |
| CORPEN            | Committee of Orientation for Practices Respectful of the Environment. The CORPEN diagnostic methodology is widely used in France to characterise and mitigate the risk of pesticide transfers to groundwater and surface waters.   |
| DEM               | Digital Elevation Model  |
| DT50              | Dissipation half-life  |
| EU                | European Union   |
| FDC               | Flow Duration Curve = CDF of river discharge for a given time period (e.g. calendar month)   |
| FOCUS             | Forum for the Coordination of Pesticide Fate Models and their Use  |
| FOOT-CRS          | FOOTPRINT Catchment and Regional Scale Tool  |
| FOOT-FS           | FOOTPRINT Farm Scale Tool  |
| FOOT-NES          | FOOTPRINT National and EU Scale Tool   |
| FOOTPRINT         | Functional Tools for Pesticide Risk Assessment and Management  |
| GIS               | Geographic Information System  |
| GRDC              | Global Runoff Data Center  |
| GTOPO30           | a global DEM by USGS (United States Geological Survey) with a horizontal grid spacing of 30 arc seconds (ca. 1 km)   |
| GUI               | Graphical User Interface   |
| HOST              | Hydrology of Soil Types.<br>A delineation of UK soil types according to their hydrological properties to produce the 29-class Hydrology of Soil Types (HOST) classification. It is available as a 1km × 1 km grid.   |
| HYDRO1K           | HYDRO1K is a geographic database developed to provide comprehensive and consistent global coverage of topographically derived data sets, including streams, drainage basins and ancillary layers derived from GTOPO30.   |
| Koc               | sorption coefficient normalized to organic carbon content of the soil  |
| MACRO             | not an acronym; name relates to macropore flow.<br>MACRO is a physically-based one-dimensional numerical model of water flow and reactive solute transport in field soils. MACRO is able to simulate tile drain outflow, leaching via preferential and matrix flow, decay, plant uptake, and foliar washoff of pesticides. |
| MS                | Microsoft ®  |
| NUTS              | Nomenclature of Territorial Units for Statistics   |
| PDF               | portable document format   |
| PEC <sub>gw</sub> | Predicted Environmental Concentration in Groundwater   |
| PEC <sub>sw</sub> | Predicted Environmental Concentration in Surface Water   |
| PPDB              | FOOTPRINT Pesticide Properties Database  |
| PRZM              | Pesticide Root Zone Model.<br>PRZM is a one-dimensional, dynamic, compartmental finite-difference model that can be used to simulate chemical movement in unsaturated soil systems within and immediately below the root zone. The PRZM  |

|       |  |
|-------|--|
|       | model is able to simulate surface runoff, erosion, chromatographic leaching, decay, plant uptake, foliar washoff, and volatilisation of pesticides   |
| SGDBE | Soil Geographical Database of Europe   |
| SMU   | Soil Mapping Unit  |
| SRTM  | Shuttle Radar Topography Mission.<br>The NASA Shuttle Radar Topographic Mission (SRTM) has provided digital elevation data (DEMs) for over 80% of the globe (60° N to 56° S). These data are currently distributed free of charge by USGS and are available for download. The SRTM data are available as 3 arc second (approx. 90m resolution) DEMs. |
| STU   | Soil Typological Unit  |
| TER   | Toxicity/Exposure Ratio  |
| WFD   | Water Framework Directive, 2000/60/EC  |

## 9.2 Technical terms

| Technical term                        | Description  |
|---------------------------------------|--|
| bound residues                        | also: non-extractable residues (NER)<br>Bound residues represent compounds in soils, plants or animals which persist in the matrix in the form of the parent substance or its metabolite(s) after extraction. The extraction method must not substantially change the compounds themselves or the structure of the matrix. (Führ et al., 1998)   |
| catchment                             | A catchment (also called drainage basin or watershed) is a region of land where water from rain or snowmelt drains downhill into a body of water, such as a river, lake, dam, estuary, wetland, sea or ocean. The drainage basin includes both the streams and rivers that convey the water as well as the land surfaces from which water drains into those channels. Each catchment basin is separated topographically from adjacent catchments by a ridge, hill or mountain, which is known as a water divide. |
| dispersion                            | Dispersion is the process of solute mixing due to different travel lengths and travel times of molecules. Dispersion occurs in several media (e.g. in soils, rivers etc.) and at several scales. It increases with lateral scale and travel distance. Dispersion causes sharp solute fronts to blur, and solute breakthrough curves to broaden, flatten and develop a tail. The process of dispersion is not to be confused with molecular diffusion, which is driven by concentration gradients.                |
| FOOTPRINT agro-environmental scenario | unique combination of a FOOTPRINT soil scenario, climate scenario and climate-specific agronomic scenario  |
| mitigation                            | In the context of FOOTPRINT, this term is used in a broad sense synonymously to “risk reduction”. Hence, pesticide mitigation comprises all measures that lead to a lower risk to the environment or human beings due to pesticides. This would include also switching to another pesticide with more favourable physical/chemical or ecotoxicological properties.   |
| projection                            | A map projection is any method used in cartography to represent the two-dimensional curved surface of the earth or other body on a plane. The term "projection" here refers to any function defined on the earth's surface and with values on the plane, and not necessarily a geometric projection. There are several different types of projections, e.g. cylindrical, conic and azimuthal projections.  |

|                   |  |
|-------------------|--|
| remote sensing    | In the broadest sense, remote sensing is the measurement or acquisition of information of an object or phenomenon, by a recording device that is not in physical or intimate contact with the object. In practice, remote sensing is the utilization at a distance (as from aircraft, spacecraft, satellite, or ship) of any device for gathering information about the environment. |
| satellite imagery | Satellite imagery consists of images of Earth or other planets made from artificial satellites. Satellite images have many applications in agriculture, geology, forestry, regional planning, education, intelligence and warfare. Images can be in visible colours and in other spectra. Also elevation maps can be created from satellite images, usually made by radar imaging.   |

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**FOOTPRINT**

**Functional Tools for Pesticide Risk Assessment and Management**

**Specific Targeted Research Project**

**Thematic Priority: Policy-orientated research**

*Deliverable DL15c*

**Software specification of FOOT-NES - The national and EU-scale tool**

Stefan Reichenberger, Martin Bach

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| <b>PU</b>  | Public  | <b>X</b> |
| <b>PP</b>  | Restricted to other programme participants (including the Commission Services)        |          |
| <b>RE</b>  | Restricted to a group specified by the consortium (including the Commission Services) |          |
| <b>CO</b>  | Confidential, only for members of the consortium (including the Commission Services)  |          |

# Software Requirements Specification Document

## FOOT-NES – The national scale system

### Version 1.2 (February 2007)

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## Executive Summary

This document provides a software specification of the FOOT-NES (national and EU scale) tool. It details how the individual parts of the software, developed by different institutions within the consortium, will interface. It also provides a description of the purpose and functionality of the developed software.

FOOT-NES is mainly targeted at decision and policy makers, but has also relevance to the registration context. The tool will have the potential to support the pesticide registration authorities and the crop protection industry for higher-tier modelling purposes.

FOOT-NES will

- calculate PEC<sub>sw</sub> in (hypothetical but realistic) edge-of-field water bodies
- calculate PEC<sub>gw</sub> at 1 m depth (regulatory-relevant depth)
- facilitate ecological risk assessment for edge-of-field surface water bodies
- identify vulnerable areas (i.e. areas with a high potential risk of contamination due to soil, subsoil and climate characteristics)
- help to decide which actives should not be used in situations represented by certain agro-environmental scenarios
- perform prospective exposure assessment
- enable probabilistic exposure assessment by aggregating over given regions or countries

FOOT-NES will be coded as an extension to the ArcGIS software by ESRI, and will be compatible with both ArcGIS 9.x and 10. The tool will use the Spatial Analyst extension of ArcGIS. FOOT-NES will be developed using MICROSOFT (MS) Visual Basic Version 6.0 (with Service Pack 6) as the software language, with Visual Studio 6 as the developing tool. Some scripts will also be developed in VBA that allows an easiest development within ArcGIS. User interfaces will be available in English, French and German.

FOOT-NES will be developed as a collection of modules to be used sequentially. The FOOT-NES modules and functions will be accessible as menus in a dedicated toolbar in ArcMap.

The reliability and usability of the FOOT-NES tool will be assessed through a substantial programme of bench and beta testing, and of evaluation studies of the tool's predictive capability.

## **1 INTRODUCTION**

### **1.1 Purpose of this document**

Careful descriptions of the user requirements are the key to developing software efficiently that will be functional, useful and robust. This is critical to the design and development of software that must meet strict functionality and quality criteria. This document is applicable to the FOOT-NES system (ArcGIS extension) which is being developed by an international consortium of European researchers as part of the FOOTPRINT (Functional tools for pesticide risk assessment and management) project (Project #022704) funded by the EU via the Sixth Framework Programme.

This document will detail how the individual parts of the software, developed by different institutions within the consortium, will interface. It will also provide a description of the purpose and functionality of the developed software.

As software development is an evolving process this document will develop as the project progresses such that, when the software is complete, it will also provide a record of the design and development process. Information on the revision of this document can be found in Section 8 'Document Management'.

### **1.2 Document scope**

This specification description applies to V1.0 of the software developed 2006-2008. It is intended for use by the research consortium to clarify the development process and to serve as a description of the development process undertaken for other interested parties. It is not intended that this document should provide guidance for end users.

## **2 GENERAL DESCRIPTION**

### **2.1 Primary function of FOOT-NES**

FOOT-NES is the national and EU-scale tool and will be available as an ArcGIS extension. FOOT-NES is mainly targeted at decision and policy makers, but has also relevance to the registration context. The tool will have the potential to support the pesticide registration authorities and the crop protection industry for higher-tier modelling purposes.

The main objectives of the FOOT-NES tool are to:  
identify those areas in the EU or a member state that are most at risk from pesticide contamination  
assess the probability of pesticide concentrations exceeding legal or ecotoxicologically-based thresholds at the national or EU-scale.

The estimation of pesticide concentrations due to leaching, drainage and surface runoff/erosion will rely on the deterministic models MACRO and PRZM while simpler, more pragmatic approaches (e.g. drift calculation formulae according to FOCUS) will be used for assessing pesticide inputs via spray drift. More details are given in Chapters 4 and 5. Predicted concentrations in surface water will allow risk assessments to be performed for aquatic taxa as FOOT-NES will include a database of ecotoxicological threshold values for fish, invertebrates, higher aquatic plants and algae.

The user will have the option to use the FOOTPRINT meta-models of MACRO and PRZM or the real models themselves. However, it is most likely that calculations encompassing the full range of scenarios (e.g. for screening purposes, or for nation- or EU-wide probabilistic exposure assessments) will be feasible only using the meta-models.

## 2.2 Relationship to the other FOOT tools (FOOT-CRS and FOOT-FS)

As part of the FOOTPRINT project two other tools will be developed in parallel to FOOT-NES. These will work at the catchment and regional scale (FOOT-CRS) and at the farm scale (FOOT-FS). The three tools will be complementary and tailored to the different needs of the different user groups (cf. section 2.3). Redundance of information or inconsistencies between the tools are therefore to be avoided. However, the three tools will share the same overall philosophy and underlying science, and also some facilities and auxiliary tools such as the FOOTPRINT PPDB. While FOOT-NES and FOOT-FS will calculate Predicted Environmental Concentrations in surface water (PEC<sub>sw</sub>) for edge-of-field water bodies, the FOOT-CRS tool will calculate PEC<sub>sw</sub> at catchment outlets.

In contrast to FOOT-CRS and FOOT-FS, FOOT-NES will not deal with point sources. Since data availability on point sources is low at those large scales, and point sources have to be mitigated against at farm and catchment scale, it was not deemed meaningful to include point source calculations into FOOT-NES.

Another difference to FOOT-FS and FOOT-CRS is that exposure/risk assessment in FOOT-NES is meant to be exclusively prospective. If the user wants to conduct an exposure/risk assessment for a concrete, real situation, the user is referred to the two smaller-scale tools.

Both FOOT-NES and FOOT-CRS are conceived as ArcGIS extensions. The development of both tools shall be as close and harmonized as possible to ensure scientific and technical consistency. FOOT-CRS and FOOT-NES will share large parts of their code and their modular structure.

The range of mitigation measures included will be different for the three tools, corresponding to their different scales.

## 2.3 Characterisation of end-users and their needs

FOOT-NES is expected to be predominantly used by policy and decision makers, e.g. ministry officials or EU DG ENV members. However, the tool is also potentially useful to regulatory authorities and the crop protection industry.

Each of these potential user groups will have different needs with respect to system design, data input and the presentation of model results. However, these needs will be less different than between the potential user groups of the farm-scale tool FOOT-FS. Computer literacy of different potential end-users may vary, but can be expected to be generally higher than for FOOT-FS users. It will be necessary to ensure that the user interface is sufficiently flexible in functionality to meet the needs of each group. Data input will need to be streamlined, efficient and simple to operate and the system output will need to be presented to the user in a format that is at an appropriate level of detail to match their needs. The possibility of errors due to wrong GIS handling has to be minimized.

### 2.3.1 Policy and decision makers

#### *User objectives:*

- To identify those areas in the EU or in a member state that are most vulnerable to the contamination of water resources by the agricultural use of pesticides.
- To aid the development of policies and legal frameworks which will help limiting the transfer of pesticides to surface water and groundwater bodies and moving towards an ecologically and economically sustainable agriculture in the EU. For instance, FOOT-NES may be used for a priori evaluation of policies.
- To aid the implementation of existing legislation in the context of pesticide risk management (e.g. implementation of the Water Framework Directive 2000/60/EC)
- To play with what-if scenarios to assess the impact of changing agricultural policies etc.
- To devise/design national or EU-wide monitoring programmes
- To identify locations for more complex or smaller-scale modelling



*User limitations:*

- Not all users may be familiar with the use of GIS or remote sensing data, hence the need for good tool support and tutorials.
- Likely to be more familiar with active substances than brands.
- May need support for selecting pesticide properties
- May need support for specifying pesticide application schemes.

*User interface needs:*

- Quick to operate.
- integrate well into the ArcGIS user interface
- easy and safe replacement of default spatial data with better-resolved spatial data provided by the user
- Moderate levels of user support and help.
- Tools for providing access to pesticide properties.

*Results presentation requirements:*

- Optional full access to model hard data.
- Powerful reporting facilities (maps, reports, figures, statistics)
- Colour-coded output maps for communication with non-experts

### 2.3.2 Regulators and crop protection industry

*User objectives:*

- To identify the pathways and those areas in the EU or a member state that contribute most to the contamination of water resources by the agricultural use of pesticides.
- To perform large-scale screening of substances for risks to surface water and groundwater resources all over Europe (EU-25 and Member States)
- To conduct a refined (“higher-tier”) exposure assessment, e.g. under consideration of kinetic sorption, metabolites or certain mitigation measures
- To identify regulatory-relevant mitigation strategies to reduce the risk resulting from pesticide inputs into surface water and groundwater bodies to an acceptable level.
- To provide probabilistic and georeferenced probabilistic exposure/risk estimates
- To design and optimise national monitoring programmes (sampling points, sampling times and intervals, analysed substances)
- To support post-registration risk management

*User limitations:*

- Very limited in time resources.

*User interface needs:*

- Quick to operate.
- integrate well into the ArcGIS user interface
- easy and safe replacement of default spatial data with better-resolved spatial data provided by the user
- Moderate levels of user support and help.
- Sophisticated data input options for higher-tier exposure assessment.

*Results presentation requirements:*

- Optional full access to model hard data.
- Powerful reporting facilities (maps, reports, figures, statistics)

## 2.4 What will FOOT-NES do / not do?

The following discusses the capabilities and limitations of FOOT-NES.

### *Mitigation*

FOOT-NES will be able to assess the effect of a number of mitigation measures at the national and EU scale. It will be able to give recommendations which mitigation measures that can be implemented nation- or EU-wide must be chosen to manage the risk of pesticide contamination of water resources at the member state or EU level. At this scale, the main control is the authorisation of active ingredients or products. Hence, the relevant mitigation measures for national and EU scale are usage restrictions (e.g. with respect to maximum application rates, application periods, certain crops or soil types) and prescription of minimum distances (no-spray buffers) and vegetative buffer strips (such as grassed buffers at the lower edges of fields against surface runoff and erosion).

### *Monitoring*

FOOT-NES will support the design of broad national and EU-wide monitoring campaigns. However, FOOT-NES is not suited for the development of targeted monitoring campaigns with higher sampling frequencies at the catchment scale. For this purpose, the user is referred to the FOOT-CRS tool.

### *Risk Assessment and Management*

FOOT-NES will:

- calculate PEC<sub>sw</sub> in (hypothetical but realistic) edge-of-field water bodies
- calculate PEC<sub>gw</sub> at 1 m depth (regulatory-relevant depth)
- facilitate ecological risk assessment for edge-of-field surface water bodies
- identify vulnerable areas (i.e. areas with a high potential risk of contamination due to soil, subsoil and climate characteristics)
- help to decide which actives should not be used in situations represented by certain agro-environmental scenarios
- perform prospective exposure assessment
- enable probabilistic exposure assessment by aggregating over given regions or countries

FOOT-NES will NOT:

- calculate PEC<sub>sw</sub> at catchment outlets
- provide exact, numerical pesticide concentrations in groundwater bodies. Instead, model results at 1 m depth will be considered together with groundwater vulnerability information (cf. Højberg et al., 2006) to identify areas with high risk for groundwater bodies.

### *Point sources*

Point sources are an important input pathway for pesticides into water bodies. However, data availability on point sources is low at these large scales, and point sources have to be mitigated against at farm and catchment scale anyway. Hence, it was not deemed meaningful to include point source calculations into FOOT-NES.

### *“What-if” calculations with respect to climate change*

At the Annual Meeting in Copenhagen (23-24 Nov 2006) it was suggested to, since both climate and land use can change quite quickly (the latter due to changes in climate, markets and policies), facilitate “what-if” calculations with the FOOT tools. This way future exposure situations could be assessed and feed into current planning. Importing future land use scenarios into FOOT-NES is possible. Introducing new climate scenarios (i.e. new weather time series) implies that the meta-models included in FOOT-NES cannot be used for calculations, and thus the real MACRO and PRZM models will have to be run. The user will be given the opportunity to do this, but the

necessary computation time is expected to be very long, depending on the number of agro-environmental scenarios and pesticide application scenarios selected.

### *Kinetic sorption*

FOOT-NES will offer the possibility to simulate kinetic sorption for the purpose of higher-tier exposure assessment. However, this requires the use of the real MACRO model as opposed to the meta-model. Therefore, depending on the number of agro-environmental scenarios and pesticide application scenarios selected for simulation, the necessary computation times may be very long.

### *Uncertainty issues*

The predictive capability of FOOT-NES will be assessed in a number of evaluation studies (cf. section 7.1).

Each output of FOOT-NES to the user will be accompanied with a qualitative or (where possible) quantitative statement of uncertainty. The limitations of the tool will be documented in the User Manual and mentioned in the FOOT-NES output wherever necessary.

At least in the later versions of FOOT-NES, Module 4 (Pesticide Scenarios) and Module 6 (Mitigation Manager) will contain an uncertainty/variability processor for the purpose of probabilistic exposure assessment, and to provide a more reliable basis for decision-making. However:

- FOOT-NES will not include facilities for Monte Carlo sampling. Thus, input parameter sets will have to be provided by the user.
- The interpretation of output distributions will have to be done by the user himself outside FOOT-NES.

At the moment, the uncertainty/variability processors are of lower priority than the core functionalities of the FOOT tools. Hence, the first version of FOOT-NES will probably not contain these processors due to time constraints.

## **3 SOFTWARE DEVELOPMENT**

### **3.1 Overview of development process**

The present System Specification document seeks to describe the purpose, functionality and the technical aspects of the tool including its objectives, end-users, programming language, system modules and data exchange. From this document a detailed design phase is undertaken which describes the system data flow, user interface (both data input and results output) and user facilities in terms of both their technical nature and end presentation. The software coding phase converts the scientific processes developed with the FOOTPRINT project into functional software. Databases will be developed and populated. Once the basic tool is developed it will undergo extensive in-house bench testing before the beta versions are released for testing and workshop evaluations are undertaken. Finally, based on the outcomes and findings of the piloting and evaluation process the software is debugged, refined and finalised.

### **3.2 Development languages, tools and platforms**

#### *Software*

FOOT-NES will be coded as an extension to the ArcGIS software by ESRI, and will be compatible with both ArcGIS 9.x and 10. The tool will use the Spatial Analyst extension of ArcGIS. FOOT-NES will share a lot of code with FOOT-CRS to ensure consistency.

FOOT-NES will be developed using MICROSOFT (MS) Visual Basic Version 6.0 (with Service Pack 6) as the software language, with Visual Studio 6 as the developing tool. Some scripts will also be developed in VBA that allows an easiest development within ArcGIS.

User interfaces will be available in English, French and German, which are the most widely used languages in the EU. The VB6 development platform will be enhanced by the addition of a module designed to provide multi-lingual support. This is 'Multi-Language Add-In' available from Softwarebuero Jollans ([www.jollans.com](http://www.jollans.com)). This company develops software for technical applications such as VB and this tool provides a general solution for creating and maintaining multilingual versions of VB6 projects. The advantage of this approach is that just one version of the software is developed and translation of the strings is embedded into the software code. The module requires the software engineer to develop language dictionaries that holds the required language translations in all text used within the software program.

In addition to the main FOOT-NES software package a number of databases will be fully integrated and used for the storage and retrieval of meta-model data, agro-environment scenario descriptions, pesticide properties data (cf. section 6.1) and language dictionary elements (section 6.2). The same databases will be common to the 3 tools. The databases will be developed and managed using Microsoft Access 2003 software package and the Access 2000 file structure. MS Access 2003 is a database-management system that allows one to create, edit, organise, store and retrieve databases in a variety of different ways. This version of Access has been selected because it is robust and will support the Greek character set and fonts (which are necessary for FOOT-FS, not for FOOT-NES or FOOT-CRS).

### *Operating systems and hardware*

FOOT-NES will be designed and developed to operate on both the Windows 2000 and Windows XP platforms. Possibly the software will also work with older Windows versions, but only if ArcGIS actually runs on them.

The optimal and minimum hardware requirements for FOOT-NES will be identified during the System Performance bench testing exercises (see Section 7.3).

## **4 GENERAL FUNCTIONAL REQUIREMENTS**

### **4.1 System shell**

FOOT-NES will be developed as a collection of modules to be used sequentially. These modules will be accessible as menus in the ArcGIS Graphical User Interface.

The advantage of a modular approach is that it is memory efficient allowing the software to work on less powerful computers as only the module being operated is open and utilising computer memory at any one time. It also allows the risk assessment process to be carried out in stages rather than as a single exercise. It also enables easier and more efficient software maintenance.

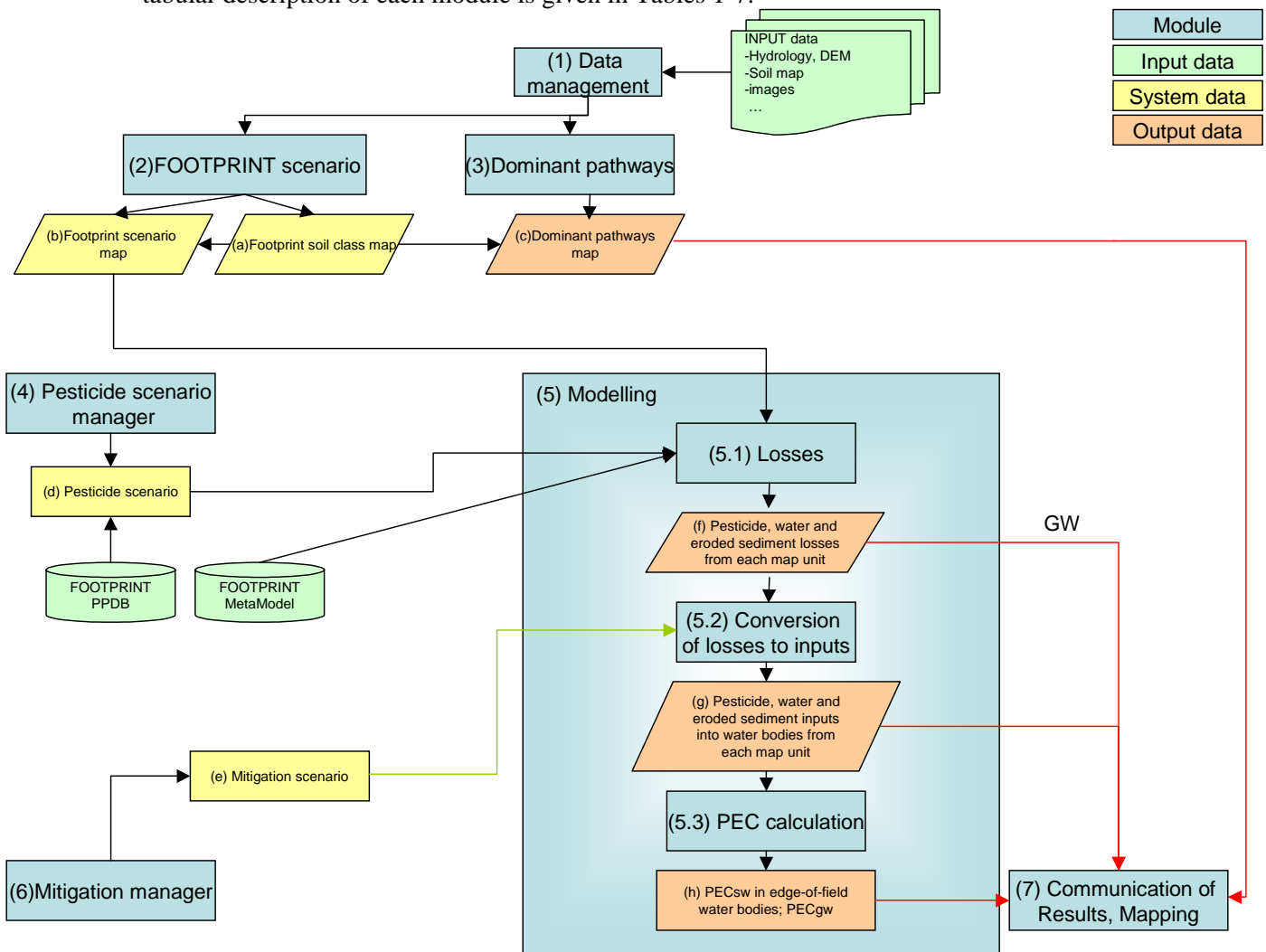
### **4.2 What the system must accomplish**

The system must:

- Meet the objectives of FOOT-NES (see Section 2.1).
- Harmonise with the other FOOT-tools (see Section 2.2)
- Integrate well with the ArcGIS software
- Meet the needs of all end-users in terms of functionality, performance and integrated user support (see Section 2.3).
- Be available in English, German and French.
- Be maintainable and capable of being upgraded as simply and quickly as possible.

### 4.3 The system core and architecture

The schematic diagram below (Figure 1) shows the general FOOT-NES structure and flow of information. The software is broken down into 7 modules with different functions. A detailed tabular description of each module is given in Tables 1-7.



**Figure 1. Schematic diagram of the FOOT-NES structure and information flow.**

#### Explanations

Manager: user interface that allows to add/modify/delete data (mainly geographic data)

System data: internal data; i.e. the user does not have direct access to them as opposed to input/output data.

- a) FOOTPRINT soil class map
- b) FOOTPRINT scenario map (FOOTPRINT “scenario” = FOOTPRINT agro-environmental scenario)
- c) Dominant pathways map
- d) Pesticide scenarios (compound + application)
- e) Mitigation scenario(s).
- f) Maps of pesticide, water volume and eroded sediment losses from each map unit
- g) Maps of pesticide, water volume and eroded sediment inputs into water bodies from each map unit
- h) PEC<sub>sw</sub> in edge-of-field water bodies; PEC<sub>gw</sub>

|                  |  |           |
|------------------|--|-----------|
| <b>Module</b>    | <b>Data management</b>   | <b>M1</b> |
| <b>Objective</b> | The user can manage the data layers of FOOT-NES  |           |
| <b>Interface</b> | Data management window   |           |
| <b>Input</b>     | All default and user data (1)  |           |
| <b>Functions</b> | Import<br>Add/remove<br>Replace (to a certain extent)<br>Metadata description (source, scale...) |           |
| <b>Output</b>    | Dataset formatted in a usable way,<br>Data description in internal DB                            |           |

**Table 1a. The “Data Management” module.**

| (1) Dataset   | Geographic | Default  | Can be replaced by the user | Comments   |
|---|------------|--|-----------------------------|--|
| FOOTPRINT soil map  | Yes        | European soil Data Base                        | Yes                         |  |
| DEM   | Yes        | HYDRO-1K                                       | Yes                         |  |
| FOOTPRINT agronomic scenario map                                  | Yes        | Corine land cover                              | Yes                         |  |
| Administrative boundaries   | Yes        | Nuts2 map                                      | Yes                         |  |
| FOOTPRINT climatic scenario map                                   | Yes        | Grid from WP2                                  | NO                          |  |
| Surface water network   | Yes        | CCM2   | Yes                         |  |
| Catchment boundaries and outlet location                          | Yes        | CCM2   | Yes                         |  |
| area-specific daily discharge                                     | Yes        | data from GRDC in Koblenz                      | Yes                         | either monthly means or Flow Duration Curves (FDC) |
| Layers used for GW vulnerability assessment                       | Yes        |  | Yes                         | TBD by Anker within WP2                            |
| Compounds DB  | No         | Footprint PPDB                                 | No                          |  |
| Metamodel DB  | No         | Footprint MM                                   | No                          |  |
| Drainage map (artificially drained percentage of the arable land) | Yes        | Estimate based on region and HOST-CORPEN class | Yes                         | To be done.  |

**Table 1b. Input data for FOOT-NES.**

| Module                     | FOOTPRINT Scenario  | M2 |
|----------------------------|---|----|
| <b>Objective</b>           | Module that provides the map of FOOTPRINT soil classes and FOOTPRINT scenarios (either take default or facilitate map creation from user data)  |    |
| <b>Interface</b>           | Button “Create scenario map” in the main toolbar  |    |
| <b>Input</b>               | Soil maps, climatic scenario map, Area of Interest (country boundaries), DEM, Land use.<br>Scenario definition  |    |
| <b>Functions / actions</b> | Create FOOTPRINT scenario map (This will only be necessary if the user wants to use his own input data. The FOOTPRINT default scenario maps will have been created beforehand and will be included in the software CD/DVD.) |    |
| <b>Output</b>              | Map of FOOTPRINT soil Classes<br>Map of FOOTPRINT Scenario  |    |

**Table 2. The “FOOTPRINT Scenario” module.**

| Module                     | Dominant pathways  | M3 |
|----------------------------|--|----|
| <b>Objective</b>           | Create the dominant pathways map<br>The map of dominant pathways will state whether an area is more likely to pesticide losses to surface water (via surface runoff/erosion, subsurface flow or drainflow) to groundwater via leaching. The map can thus be used to assess the inherent vulnerability of groundwater and surface water resources within the EU.  |    |
| <b>Interface</b>           | Button “Create dominant pathways map” in the main toolbar  |    |
| <b>Input</b>               | Footprint soil classes map, DEM and surface water network<br>IDPR algorithm  |    |
| <b>Functions / actions</b> | Identification of the main contamination pathways through an innovative, data-parsimonious methodology referred to as the "Index of development and persistence of hydrological networks" (IDPR) recently developed at BRGM. The methodology yields the natural tendency of a given area to let water infiltrate or to transfer water to an adjacent surface water body.<br>Create dominant contamination pathways map (DEM cells as map units). |    |
| <b>Output</b>              | Map of dominant contamination pathways   |    |

**Table 3. The “Dominant Pathways” module.**

| Module                     | Pesticide scenario manager   | M4 |
|----------------------------|--|----|
| <b>Objective</b>           | Allows the user to define and manage the pesticide scenario  |    |
| <b>Interface</b>           | Pesticide scenario window  |    |
| <b>Input</b>               | <ul style="list-style-type: none"> <li>- Footprint Crop list</li> <li>- Footprint PPDB</li> </ul>  |    |
| <b>Functions / actions</b> | <ul style="list-style-type: none"> <li>- User input of the following parameters.</li> <li>- active substance (select from PPDB or enter own DT50/Koc)</li> <li>- crop,</li> <li>- application date</li> <li>- application rate</li> <li>- % of crop treated</li> <li>- Possibility to apply pesticide to more than one crop; then repeat steps above for the other crops.</li> </ul> |    |

|               |  |
|---------------|--|
|               | <ul style="list-style-type: none"> <li>- Option 1: Unique parameter values for the whole area of interest, then the user selects a value in a combo-box for each parameter.</li> <li>- Option 2 : For some parameter (e.g. application rate, application month, % of crop treated), the value can be localized. For each parameter, the user can:</li> <li>- Create a new “&lt;parameter&gt; map”, from an existing Vector layer</li> <li>- assign a &lt;parameter&gt; value to each polygon. (from an predefined list of choice)</li> <li>- The user can manage (new, save, modify, delete) the scenarios.</li> <li>- In the later versions of FOOT-NES, the module will contain an uncertainty/variability processor.</li> </ul> |
| <b>Output</b> | Pesticide scenarios list in DB<br>Parameters of each scenario in DB  |

**Table 4. The “Pesticide Scenario Manager” module.**

| Module                     | Modelling  | M5 |
|----------------------------|--|----|
| <b>Objective</b>           | Compute maps and distributions of PEC (or any other output variables)  |    |
| <b>Interface</b>           | “Perform Model” button   |    |
| <b>Input</b>               | <ul style="list-style-type: none"> <li>- area-specific discharge</li> <li>- Data for GW vulnerability assessment (TBD by Anker)</li> <li>- Footprint scenario map</li> <li>- Pesticide scenario</li> <li>- Metamodel DB</li> <li>- Mitigation scenario (none by default)</li> <li>- Modelling algorithm</li> </ul> |    |
| <b>Functions / actions</b> | The user can select a Mitigation scenario. By default, no mitigation scenario is selected.<br>Modules 5.1, 5.2, 5.3 are run successively.  |    |
| <b>Output</b>              | Pesticide input maps for each pathway<br>Results tables/figures for pesticide exposure (e.g. CDF over time and/or space).  |    |

**Table 5a. The “Modelling” module**

| Module                     | Losses modelling  | M5.1 |
|----------------------------|---|------|
| <b>Objective</b>           | Compute pesticide, water and sediment losses  |      |
| <b>Interface</b>           | “Perform Model” button  |      |
| <b>Input</b>               | <ul style="list-style-type: none"> <li>- Footprint scenario map</li> <li>- Pesticide scenario</li> <li>- Metamodel DB</li> <li>- Mitigation scenario (none by default)</li> </ul> |      |
| <b>Functions / actions</b> | For each mapping unit and contamination pathway, compute the pesticide losses (if applicable, also water and eroded sediment losses).   |      |
| <b>Output</b>              | <ul style="list-style-type: none"> <li>- Maps of pesticide, water and eroded sediments losses from each map unit.</li> <li>- Map of PECgw in 1 m depth</li> </ul>                 |      |

**Table 5b. The “Losses Modelling” sub-module.**



|                            |  |             |
|----------------------------|--|-------------|
| <b>Module</b>              | <b>Losses conversion to inputs</b>   | <b>M5.2</b> |
| <b>Objective</b>           | Compute pesticide, water and eroded sediments inputs into water bodies from each map unit  |             |
| <b>Interface</b>           | - none -   |             |
| <b>Input</b>               | Maps of pesticide, water and eroded sediments losses from each map unit.<br>Mitigation scenario (none by default)<br>Data for GW vulnerability assessment (TBD by Anker) |             |
| <b>Functions / actions</b> | For each pathway and mapping unit, convert losses from the unit to inputs into water bodies.   |             |
| <b>Output</b>              | Maps of pesticide, water and eroded sediments inputs into water bodies from each map unit.<br>Maps of pesticide concentrations in groundwater.                           |             |

**Table 5c. The “Losses Conversion To Inputs” sub-module.**

|                            |   |             |
|----------------------------|---|-------------|
| <b>Module</b>              | <b>PECsw computation</b>  | <b>M5.3</b> |
| <b>Objective</b>           | Compute PECsw in edge-of-field water bodies   |             |
| <b>Interface</b>           | - none -  |             |
| <b>Input</b>               | <ul style="list-style-type: none"> <li>- dimensions of water body: length, width, profile, water table height (changeable default provided)</li> <li>- area-specific discharge (changeable default provided)</li> <li>- Maps of pesticide, water and eroded sediments inputs into water bodies from each map</li> </ul> |             |
| <b>Functions / actions</b> | TBD; an option is to use the core of the STEPS-1-2-3-4 tool by M. Klein, IME Schmollenberg  |             |
| <b>Output</b>              | Maps of PECsw in edge-of-field water bodies<br>Results tables/figures (e.g. CDF over time and/or space).  |             |

**Table 5d. The “PECsw Computation” sub-module**

|                            |  |           |
|----------------------------|--|-----------|
| <b>Module</b>              | <b>Mitigation manager</b>  | <b>M6</b> |
| <b>Objective</b>           | Allows the user to define and manage the mitigation scenario   |           |
| <b>Interface</b>           | Mitigation manager window  |           |
| <b>Input</b>               | List of predefined mitigation measures and associated predefined parameters (these are the parameters that define the mitigation action. For instance, if the mitigation strategy is “reduction of application rate”, then “% of reduction” or “Alternative application rate” is the associated parameter.   |           |
| <b>Functions / actions</b> | <p>Some mitigation measures are “global”, e.g. change of the application date or rate. (The user chooses the nominal pesticide scenario in the Pesticide scenario Manager, and computes the results. Then he can add some mitigation measures and run the model again. The results of the simulation with mitigation measures are then compared with those of the nominal pesticide scenario).</p> <p>Some measures can be localized (e.g. buffer zones).</p> <p>The mitigation manager allows the user to define and save different mitigation scenarios.</p> <p>In the later versions of FOOT-NES, the module will contain an uncertainty/variability processor.</p> |           |

|               |  |
|---------------|--|
| <b>Output</b> | Mitigation scenarios list in DB<br>Parameters of each mitigation scenario in DB. |
|---------------|--|

**Table 6. The “Mitigation Manager” module.**

| <b>Module</b>              | <b>Display + Mapping of Results</b>  | <b>M7</b> |
|----------------------------|--|-----------|
| <b>Objective</b>           | Display results (maps and figures)   |           |
| <b>Interface</b>           | ArcGIS main window with dedicated legend button<br>Modelling result window.  |           |
| <b>Input</b>               | Maps from module 2, 3, and 5<br>Figures from module 5  |           |
| <b>Functions / actions</b> | The user can <ul style="list-style-type: none"> <li>- Display PEC maps (for each pathway), and change legend</li> <li>- Display figures (+explanatory text) from the modelling (e.g. CDF)</li> <li>- Display summary text (report).</li> <li>- Display proposed mitigation strategies</li> <li>- Export maps and reports.</li> </ul> |           |
| <b>Output</b>              | Result display<br>Exports (maps/figures as jpg/pdf; report as txt/doc/pdf)   |           |

**Table 7. The “Display + Mapping of Results” module.**

#### 4.4 Integration in ArcGIS

The FOOT-NES modules and functions will be accessible as menus in a dedicated toolbar in ArcMap. The toolbar, menus and dialogues will be very similar (partly identical) to the ones in FOOT-CRS. For further details, the reader is therefore referred to the corresponding section in FOOT-CRS software specification document.

#### 4.5 Software management

##### *Bug fixing and software upgrades post release v.1*

A software bug is an error, failure, or fault in a software program that prevents it from behaving as intended. Bugs can arise from errors made during the program coding process and/or during its design. They can have a wide variety of effects, with varying levels of inconvenience to the user of the program. Serious bugs may cause a software program to stop operating i.e. to crash or to freeze. Usually these bugs will be identified during bench and beta testing exercises. However, some bugs may only occur in very specific circumstances or only with particular data sets. These usually have only a subtle effect on the program's functionality and so may lie undetected for a long time. It is virtually impossible to test and evaluate a software program's performance with every possible set of input data or in every possible way an end user may operate it. Consequently, it is rare for a software program to be completely bug-free. Therefore it is important that procedures are put in place for end users to report bugs, for bugs to be fixed and upgrades or software patches distributed.

The FOOTPRINT website will have facilities for users to report bugs directly to the software developers and to provide (wherever possible) the input data causing the problem. This is particularly important as it is not always easy to reproduce bugs. Some bugs are triggered by inputs to the program that may be difficult for the programmer to re-create.

Once the bug has been identified and fixed a corrected version of the module at fault will be available for download from the FOOTPRINT website. Details regarding the error and bug fix will

be also logged on the website. Each new release will be given a unique version number for reference.

### *Software upgrades*

From time to time it may be necessary for scientific or technical reasons to revise the software and/or the underpinning databases. If and when this occurs a new version of the module or modules revised will be available on the FOOTPRINT website for download. Details of the upgrade, technical changes and release date will also be logged on the website. Each new release will be given a unique version number for reference.

### *Maintenance*

Maintenance and updating will be performed by Stefan Reichenberger and Martin Bach at University Giessen during the development phase. After the end of the FOOTPRINT project in December 2008 a maintenance structure will be established for all 3 tools.

## **5 THE CORE SYSTEM**

### **5.1 System Shell**

The FOOT-NES system shell will be integrated in the ArcGIS shell. It will include:

- Menus (integrated in the ArcGIS menu bar) allowing the user to navigate through the modules to complete an exposure assessment. Menu items will be direct links to the relevant modules and tools.
- Buttons to compute new information from existing data (e.g. compute a new map layer)
- Buttons to open a screen or dialogue of a module or tool (alternative path to the menus)
- Help and support including:
  - General introductory text to FOOT-NES, the other FOOTPRINT tools and the FOOTPRINT project.
  - General help text regarding the operation of the FOOT-NES system and the tools and facilities available.
  - Video tutorials
  - Links to the FOOTPRINT website
  - Upgrading and updating tools showing module versions numbers, availability of upgrades and automatic upgrade functions.

FOOT-NES will consist of seven different modules (cf. Tables 1-8). Four of them will have substantial interaction with the user: three modules for data input (Data Management, Pesticide Scenario Manager, Mitigation manager), and one for model output (Display + Mapping of Results). The remaining three modules FOOTPRINT Scenario, Dominant Pathways and Modelling are just launched by the user and offer no further interaction.

### **5.2 Data input**

For all input data, there are two possibilities for the user depending on data availability:

- Use of the default FOOTPRINT scenarios (FOOTPRINT soil classes, FOOTPRINT agronomic scenarios etc.)
- Input of own data if available at a finer resolution

#### *Data Management Module*

Soil and land-use spatial data imported by the user in the Data Management module (module 1) are subsequently converted into a map of FOOTPRINT scenarios in the FOOTPRINT scenario module (module 2). To enable this, the user has to assign FOOTPRINT classes to the classes in his

own map. To aid the correct assignment of FOOTPRINT soil classes to the soil classes in the user's map, substantial descriptive text and also the soil taxonomic unit according to the FAO or the similar WRB system will be provided with each FOOTPRINT soil class.

It is proposed to use the HYDRO-1k Digital Elevation Model derived from GTOPO data (ca. 1 km resolution) as default DEM, and the CORINE land cover cells (250 m \* 250 m) as basic map units. However, the user will be able to import and use a higher-resolved DEM (e.g. derived from SRTM data with 90 m resolution) and thus also to have smaller map units.

The data import tools in module 1 must have extensive capabilities:

- automatically change the projection and datum to the FOOTPRINT standard projection and datum (although ArcGIS performs on-the-fly projection, it is safer to perform a real change of the projection)
- automatically change resolution (pixel size) by resampling
- adjust variables and classes in attribute tables to the FOOTPRINT data format
- correctly assign FOOTPRINT scenarios to variables and classes in attribute tables of imported maps (the assignment has to be done by the user, but the implementation of the assignment will be done automatically by the import tools)

### *Pesticide Scenario Manager*

In the Pesticide Scenario Manager (module 4), the user enters all pesticide-related input:

- active ingredient(s) incl. physical and chemical properties (changeable default values provided in the FOOTPRINT PPDB),
- treated crop(s),
- application rate(s),
- percentage of crop area that is treated
- application date(s).

The so created pesticide application scenarios can either be applied to the whole area of interest (EU, member states) or to only parts of it (e.g. NUTS-2 levels).

In the later versions of FOOT-NES, the module will contain an uncertainty/variability processor for probabilistic risk assessment, to evaluate the effect of variable and/or uncertain parameters in the pesticide scenarios: (compound properties, application rate and date, treated percentage of crop area).

### *Mitigation manager*

The Mitigation Manager (module 6) allows the user to define and save different mitigation scenarios. Mitigation measures for reducing pesticide inputs into water bodies can be selected from a predefined list. Changeable default values will be provided for the efficiencies of the various measures. The specified mitigation measures will be used in the "Conversion of losses to inputs" step (sub-module 5.2)

In the later versions of FOOT-NES, the module will contain an uncertainty/variability processor for probabilistic risk assessment, to evaluate the effect of variable and/or uncertain properties of mitigation features (density, position, abundance, efficiency).

## **5.3 Pre-modelling phase and meta-modelling**

Using spatial data input into the system (cf. Table 1b), the software will i) assign FOOTPRINT scenarios to areas in the EU or a member state (Module 2), and ii) using the innovative and data-parsimonious IDPR methodology, calculate coherent maps of dominant contamination pathways (Module 3). These maps tell whether a particular area is likely to contribute to groundwater recharge or surface or subsurface runoff to surface water. Pesticide property data required to drive

the meta-models of MACRO and PRZM (or, for what-if or higher-tier calculations, MACRO and PRZM themselves) will be identified and retrieved from the PPDB (see Section 6.2).

### *Assigning scenarios to areas (FOOTPRINT map units)*

With the Europe-wide default data sets provided by FOOTPRINT the agro-environmental scenarios cannot be localized exactly, because:

A soil mapping unit (SMU) in the Soil Geographical Database of Europe (SGDBE) has a distribution of soil scenarios (FOOTPRINT soil classes) with different area proportions or probabilities of occurrence each (e.g. 40 % soil A, 20 % soil B etc.).

A crop mapping unit from CLC2000 has a distribution of crops with different area proportions or probabilities of occurrence each (e.g. 40 % winter wheat, 20 % winter barley, 20 % maize etc.), which are given by the NUTS-2 level agricultural statistics.

Each FOOTPRINT map unit has exactly one climate scenario, but an area distribution of crops, soils and thus of “agro-environmental scenarios”. As a consequence, scenarios and thus simulated pesticide losses will be assigned to the areas in the EU or country statistically, using the following assumptions:

The areic distribution of FOOTPRINT soil classes is homogeneous over the SMU.

The areic distribution of crops is homogeneous over the agricultural census unit (which is not realistic at NUTS-2 level).

If there are unrealistic crop/soil combinations in a FOOTPRINT map unit (e.g. potatoes on a heavy clay), the area of this combination is assumed as zero. The area of the crop is then redistributed proportionally to the other soil classes in the FOOTPRINT map unit.

If the user has his/her own, better resolved soil and/or land use data with only one scenario per soil mapping unit and/or land-use mapping unit, respectively, the assignment of scenarios to FOOTPRINT map units will be considerably easier.

### *Calculate map of dominant contamination pathways*

The Dominant pathways module (module 4) aims at creating a map of dominant contamination pathways. This map will state whether an area is more prone to pesticide losses to surface water bodies (via surface or subsurface runoff and erosion) or to groundwater via leaching.

This aim will be achieved by combining information from

- the FOOTPRINT soil scenarios map and
- application of the IDPR methodology

IDPR (“Index of development and persistence of hydrological networks”) is an innovative, data-parsimonious methodology which yields the natural tendency of a given area to let water infiltrate or to transfer water to an adjacent surface water body. The general principle of the methodology is a comparison between the existing hydrological network for a given area and a theoretical hydrological network created from a digital terrain model. The deployment of IDPR at EU scale will result in a coherent map telling whether a particular area is likely to contribute to groundwater recharge or runoff to surface water. This map can be used to assess the inherent vulnerability of groundwater and surface water resources within the EU.

The dominant contamination pathways for each map unit will be computed for two seasons (field capacity period and soil moisture deficit period based on the FOOTPRINT soil map) and be displayed in a colour-coded format. It has to be kept in mind (and will be explicitly communicated to the user) that this information is only qualitative, and that the absolute and relative contributions of the different pathways to pesticide contamination of water resources can vary dramatically from year to year.

## 5.4 Modelling and meta-modelling

Mathematical modelling is the process of creating a simplified mathematical representation of a real-world process in order to gain a better understanding of it. It is a process which attempts to match observation with a mathematical description. During the process of building the model, in order to simplify the mathematical representation, the developer must decide what factors are relevant to the problem and what factors can reasonably be ignored. The consideration and incorporation of more factors may well improve the models performance, but this is often a trade-off against the models run-time and the computing power required for its operation. For scientists, policy makers and regulators long model run-times of 1 or more hours with a complex model may be acceptable, but at the national or EU scale, where thousands of model runs might be necessary, the required computation time would definitely be too long. Therefore, a meta-model approach is followed in FOOT-NES. This requires model simulations (MACRO and PRZM) to be run beforehand for all potential combinations of FOOTPRINT agro-environmental scenarios and pesticide property data (normalized sorption coefficient Koc and soil dissipation half-life DT50).

From the MACRO and PRZM simulations, 20-year daily time series for water fluxes and pesticide losses will be available for:

- Leaching at 1 m depth (MACRO)
- Drainage (MACRO)
- Infiltration excess runoff (PRZM)
- Saturation excess runoff (MACRO or PRZM; still to be decided)
- Subsurface flow (MACRO)

Since the time series themselves cannot be distributed with the software due to storage issues, meaningful summary statistics must be derived and provided with the tools. Which summary statistics (min, max, median, mean, a number of percentiles etc.) have to be stored and distributed with the software depends on the PEC calculation methods and on user needs. It is furthermore being discussed whether various pesticide loss percentiles for the whole time series are sufficient or loss percentiles for each calendar month are needed.

The selected results from the meta-modelling exercises will then be formatted into look-up tables and stored as a suite of MS Access database files. Data from these will be retrieved based on the Koc and DT50 of the pesticide being modelled. The pesticide Koc and DT50 will be retrieved directly from the FOOTPRINT PPDB (see Section 6.1) although facilities will be incorporated to override this default with the users own data.

It will however be possible for the user to perform simulations for selected scenarios with the real MACRO and PRZM models as opposed to the meta-models. This is relevant when e.g. nonlinear and/or kinetic sorption or formation and fate of metabolites are to be simulated. The user will also have the opportunity to export MACRO or PRZM input databases/files for each scenario, e.g. for the purpose of modelling modified, non-FOOTPRINT runs with the standalone versions of MACRO and PRZM.

## 5.5 Exposure assessment

Using the results from the meta-modelling and landscape analysis activities, the predicted environmental concentrations (PEC) in edge-of-field surface water bodies and groundwater will be calculated (Module 5). Concentrations will be estimated considering potential dilution effects based on the size and discharge of the water body, water volumes associated with runoff and drainage inputs and the presence of bed sediment.

The main outputs will be annual average leachate concentrations at 1 m depth (“PEC<sub>gw</sub>”), and PEC<sub>sw</sub> distributions in edge-of-field water bodies separately for each input pathway.

A tentative methodology for exposure assessment in FOOT-NES is provided below.

### 5.5.1 Surface water exposure assessment for edge-of-field water bodies

Compared to FOOT-CRS, calculation of Predicted Environmental Concentrations in surface water (PEC<sub>sw</sub>) and risk assessment are relatively straightforward in FOOT-NES and FOOT-FS, since only „edge-of-field“ water bodies are considered. However, FOOT-NES must also be able to provide time-weighted average concentrations (TWAC) in surface water to enable comparison with certain ecotoxicological thresholds.

It is proposed to estimate loads and PEC<sub>sw</sub> separately for each input path. For instance, surface runoff might lead to higher peak concentrations, but to less frequent exceedances of a given ecotoxicological threshold concentration than drift inputs. Having the PEC separately for each pathway will also make it easier to recommend mitigation measures and evaluate their effect at the national and EU scale. This method can be justified because the input events from the different pathways probably will not coincide on the same date.

Currently proposed general method for exposure assessment in edge-of-field water bodies (for each input path separately):

calculate pesticide (and water volume and eroded sediment, where applicable) losses from each pixel (map unit), separately for each agro-environmental scenario occurring in this pixel

- select a given percentile (X<sup>th</sup>) of the pesticide loss for each pixel, separately for each agro-environmental scenario in this pixel, and the corresponding surface runoff volume + eroded sediment or drainage volume
- convert losses to inputs into surface water
  - Drift and Runoff/Erosion: The proportions of pesticide losses from each pixel that eventually reach a water body are calculated, taking account for mitigating landscape elements between field and water body. The reduction efficiencies of the different mitigation features (e.g. buffer strips) for pesticides, runoff volumes and eroded sediment can be entered by the user. Alternatively, default efficiencies adapted from the results of FOOTPRINT DL#7 (Reichenberger et al., 2006) can be used. Without mitigation measures, runoff and erosion losses from a pixel are set equal to inputs into a surface water body from this pixel.
  - Drainage: We assume that all pesticide molecules which enter the drains will reach the surface water bodies.
- Feed these inputs into the PEC<sub>sw</sub> calculation submodule (e.g. the core of the STEPS-1-2-3-4 tool). The result is an X<sup>th</sup> percentile PEC<sub>sw</sub> for an edge-of-field water body.
- Repeat steps 2.-4. for other percentiles of the input time series (e.g. min, 5<sup>th</sup>, 10<sup>th</sup>, 20<sup>th</sup>, 25<sup>th</sup>, 30<sup>th</sup>, 40<sup>th</sup>, 50<sup>th</sup>, 60<sup>th</sup>, 70<sup>th</sup>, 75<sup>th</sup>, 80<sup>th</sup>, 90<sup>th</sup>, 95<sup>th</sup>, 99<sup>th</sup>, 99.7<sup>th</sup>, 99.9<sup>th</sup>, max).
- Read off the frequency / return period for each percentile → interpolate frequency of exceedance of a given threshold concentration

### 5.5.2 Mathematical description of exposure calculations for surface water

#### Drainage inputs

$$L_{sw,drain\_X,r} = \sum_c \sum_s \{ X^{th} \cdot \delta MACRO(STC, Climate, CropScen, AppDate) \times relDoser_{,c} \times AA\%_r \times Crop\%_{r,c,s} \times CropTreat\%_{r,c} \times STC\%_{r,s} \times AAdrain\%_r \times MFdrain\%_r \times UnitArea_r \}$$

where

$L_{sw,drain\_X,r}$  = X<sup>th</sup> percentile daily input of a.i. into surface waters via tile drains in map unit r [mg]

- $X^{\text{th}}\text{-}\delta\text{MACRO}(\text{STC}, \text{Climate}, \text{CropScen}, \text{AppDate})$  =  $X^{\text{th}}$ -percentile of the 20-year MACRO meta-model simulation results on tile drainage loss (% of dosage) of a.i. as a function of soil type class, climate, crop growth and date of application [mg/ha]
- $\text{relDoser}_{r,c}$  = application rate of a.i. to crop  $c$  in map unit  $r$ , relative to the standard rate of 1 kg ha<sup>-1</sup> of the MACRO meta-model simulation [%]
- $\text{AA}\%_r$  = Percentage of arable land, permanent cultures etc. in map unit  $r$  [%]
- $\text{Crop}\%_{r,c,s}$  = Percentage of AA on soil class  $s$  in map unit  $r$  that is cropped with field crop  $c$  [%]
- $\text{CropTreat}\%_{r,c}$  = Percentage of crop  $c$  treated with the a.i. (reflects plant protection intensity and “market share”) [%]
- $\text{STC}\%_{r,s}$  = Percentage of soil type class  $s$  in the Soil Mapping Unit [%]
- $\text{AAdrain}\%_r$  = Percentage of AA with tile drainage in map unit  $r$  [%]
- $\text{MFdrain}\%_r$  = Mitigation factor, reflecting the effects of reduction measures for tile drainage inputs from map unit  $r$  [%] (probably not relevant)
- $\text{UnitArea}_r$  = Area of the map unit  $r$  [ha]
- $r$  = Map unit index
- $c$  = Crop index (if a summation over different crops is intended, it will be necessary to calculate the loss percentiles of the MACRO/PRZM time series on a monthly basis).
- $s$  = soil class index

### Surface runoff and erosion inputs

$$\text{Lsw,runoff\_X}_{r} = \sum_c \sum_s \{ X^{\text{th}}\text{-}\delta\text{PRZM}(\text{STC}, \text{Climate}, \text{CropScen}, \text{AppDate}) \times \text{relDose}_{r,c} \times \text{AA}\%_r \times \text{Crop}\%_{r,c,s} \times \text{CropTreat}\%_{r,c} \times \text{STC}\%_{r,s} \times \text{ConF}\%_r \times \text{MFRunoff}\%_r \times \text{UnitArea}_r \}$$

where

$\text{Lsw,runoff\_X}_{r}$  =  $X^{\text{th}}$  percentile daily input of a.i. into surface waters via surface run-off and soil erosion in map unit  $r$  [mg]

$X^{\text{th}}\text{-}\delta\text{PRZM}(\text{STC}, \text{Climate}, \text{CropScen}, \text{AppDate})$  =  $X^{\text{th}}$ -percentile of the 20-year PRZM simulation results on runoff loss (% of dosage) of a.i. as a function of soil type class, climate, crop growth and date of application [mg/ha]

$\text{relDose}_{r,c}$  = application rate of a.i. to crop  $c$  in map unit  $r$ , relative to the standard rate of 1 kg ha<sup>-1</sup> of the PRZM simulation

$\text{AA}\%_r$  = Percentage of arable land, permanent cultures etc. in map unit  $r$  [%]

$\text{Crop}\%_{r,c,s}$  = Percentage of AA on soil class  $s$  in map unit  $r$  that is cropped with field crop  $c$  [%]

$\text{CropTreat}\%_{r,c}$  = Percentage of crop  $c$  treated with the a.i. (reflects plant protection intensity and “market share”) [%]

$\text{STC}\%_{r,s}$  = Percentage of soil type class  $s$  in the Soil Mapping Unit [%]

$\text{ConF}\%_r$  = Connection factor, expressing the degree of connectivity for run off and erosion input from treated fields into surface waters in map unit  $r$  [%]

$\text{MFRunoff}\%_r$  = Mitigation factor, reflecting the effects of reduction measures for pesticide run-off & erosion inputs from map unit  $r$  [%] (The two factors  $\text{ConF}\%_r$  and  $\text{MFRunoff}\%_r$  can possibly be combined.)

$\text{UnitArea}_r$  = Area of the map unit  $r$  [ha]

$r$  = Map unit index

$c$  = Crop index

$s$  = soil class index

The approach for erosion will be analogous to the one for surface runoff and is hence not listed here explicitly.



### Spray drift inputs

For 8 possible wind directions (N, NE, E, SE, S, SW, W, NW), the drift input into edge-of-field surface water bodies from a given map unit is calculated with the following formula:

$$L_{sw,drift,dir\_X,r} = \sum_c \sum_s \{ X^{th}\text{-drift\_loading}(\text{Sprayer}, \text{Distance in Wind Direction}, \text{Season}) \times \text{absDose}_{r,c} \times \text{AA}\%_r \times \text{Crop}\%_{r,c,s} \times \text{CropTreat}\%_{r,c} \times \text{MFdrift}\%_r \times \text{UnitArea}_r \}$$

where

$L_{sw,drift,dir\_X,r}$  =  $X^{th}$  percentile daily input of an a.i. into surface waters via spray drift in map unit r, for a given wind direction [mg]

$X^{th}\text{-drift\_loading}(\text{SprayerType}, \text{Distance}, \text{Season}, \text{River Width})$  = estimated  $X^{th}$ -percentile drift loading values as a function of sprayer type (boom vs. air blast sprayer, +/- drift reducing equipment), distance edge-of-field to adjacent water body, crop stage at application (early vs. late season, only for air blast applications), and river width [%]

(The choice of the distance and the percentile is left to the user.)

$\text{actDose}_{r,c}$  = application rate (actual) of a.i. to crop c in map unit r [kg/ha]

$\text{AA}\%_r$  = Percentage of arable land, permanent cultures etc. in map unit r [%]

$\text{Crop}\%_{r,c,s}$  = Percentage of AA on soil class s in map unit r that is cropped with field crop c [%]

$\text{CropTreat}\%_{r,c}$  = Percentage of crop c treated with the a.i. (reflects plant protection intensity and “market share”) [%]

$\text{MFdrift}_r$  = Mitigation factor, reflecting the effects of reduction measures for spray drift inputs from map unit r [%]

$\text{UnitArea}_r$  = Area of the map unit r [ha]

r = Map unit index

c = Crop index

s = soil class index

The variable  $X^{th}\text{-drift\_loading}$  will be calculated using the drift equation proposed by FOCUS (2001). The different percentiles will be obtained by fitting the parameters of the FOCUS drift equation to the different percentiles of the BBA drift tables (Rautmann, 2001) or of the raw data of the BBA drift trials.

The drift inputs into the surface water body for the different wind directions will be averaged using the unweighted or a weighted (with the probabilities of occurrence of the different wind directions) arithmetic mean. The weighting has to be done by the user.

Distances, drift mitigation measures and water body characteristics are also user input.

### PECsw in edge-of-field surface water bodies

No summation over input pathways is performed here, since a coincidence of peak concentrations from the different input pathways on the same day is unrealistic. PECsw for each pathway are therefore assessed separately.

It has not yet been decided on the method of PECsw and PECsed calculation; however, an option would be to use the core of the STEPS-1-2-3-4 tool by Michael Klein, IME Schmallenberg, for the calculation of edge-of-field PECsw. Step 3 and 4 of STEPS-1-2-3-4 were developed as a quick replacement for TOXSWA (FOCUS, 2001) to perform non-official FOCUSsw calculations. According to M. Klein, STEPS-1-2-3-4 yields almost the same results as TOXSWA while being much faster. A draft documentation of STEPS-1-2-3-4 is available, but the final documentation is still in preparation.

*Mathematical description of exposure calculations for groundwater*

$$PEC_{gw,1m\_X,r} = \sum_c \sum_s \{ \delta MACRO(STC, Climate, CropScen, AppDate) \times relDose_{r,c} \times AA\%_r \times Crop\%_{r,c,s} \times CropTreat\%_{r,c} \times STC\%_{r,s} \times MFleach\% \}$$

- where
- $PEC_{gw,1m\_X,r}$  =  $X^{th}$  percentile annual flux concentration of a.i. in the leachate in 1 m depth [ $\mu g L^{-1}$ ] in map unit r
  - $\delta MACRO(STC, Climate, CropScen, AppDate)$  =  $X^{th}$  percentile of annual average flux concentration from the 20-year MACRO simulation results (1 m depth) of an a.i. as a function of soil type class, climate, crop growth and date of application [ $\mu g L^{-1}$ ]
  - $relDose_{r,c}$  = application rate of a.i. to crop c in map unit r, relative to the standard rate of 1 kg  $ha^{-1}$  of the MACRO simulation [%]
  - $AA\%_r$  = Percentage of arable land, permanent cultures etc. in map unit r [%]
  - $Crop\%_{r,c,s}$  = Percentage of AA on soil class s in map unit r that is cropped with field crop c [%]
  - $CropTreat\%_{r,c}$  = Percentage of crop c treated with the a.i. (reflects plant protection intensity and “market share”) [%]
  - $STC\%_{r,s}$  = Percentage of soil type class s in the Soil Mapping Unit
  - $MFleach\%_r$  = Mitigation factor, reflecting the effects of reduction measures for leaching losses from map unit r [%] (probably not relevant)
  - r = Map unit index
  - c = Crop index
  - s = soil class index

For leaching, the PEC calculation methods are the same in FOOT-CRS and FOOT-NES. Pesticide concentrations in depths greater than 1 m will be assessed only qualitatively (cf. FOOTPRINT Deliverable DL10 (Højberg et al., 2006)).

*Database holding necessary information for exposure calculations*

| Variable  | Content, Source   | Availability  |
|---|---|---|
| $\delta PRZM(STC, Climate, CropScen, AppDate)$    |   | FOOTPRINT simulation runs                                   |
| $\delta MACRO(STC, Climate, CropScen, AppDate)$   |   | FOOTPRINT simulation runs                                   |
| STC   | Soil Type Class No., Map of Soil Mapping Units (SMU) 1:1M from SGDBE (ca. 100...150 STU), a SMU has different STC (percentages given) | FOOTPRINT soil scenarios                                    |
| Climate   | Climate scenario no. (20-y weather time series); map of European Climatic zones (ca. 15 zones)  | FOOTPRINT climate scenarios                                 |
| CropScen  | Crop growth stage scenario no. (ca. 25)   | FOOTPRINT agronomic scenarios                               |
| AppDate   | Date of application (12 or 24 dates available for selection)  | user input  |
| Xth-drift_loading (SprayerType, Distance, Season) |   | FOCUS (2001), BBA drift tables / raw data                   |
| SprayerType                                       | Type of sprayer, depends on crop type   | determined by crop, may be overridden by user in some cases |
| Distance  | distance between treated field and surface water body; for each of 8 directions (N, NE, E, SE, S, SW, W, NW)                          | user input  |
| Season  | Application season, depends on AppDate  | ---   |

|               |  |  |
|---------------|--|--|
| actDoser,c    | Actual application rate  | user input   |
| AA%r          | CORINE 2000 map (classes 211, 212, etc.); possibly needs scaling with agricultural census data due to generalization error and minimum size of mapping units | One map for EU25; can be replaced with user map  |
| Crop%r,c      | Tables: Agricultural Census on NUTS-2 level<br>Shape of NUTS-2 polygons  | EUROSTAT; can be replaced with user data   |
| CropTreat%r,c | Percentage of crop c treated with the a.i. (reflects both the plant protection intensity in that crop and catchment and the “market share”)                  | user input   |
| ConF%r        | Connectivity factor  | Can maybe be combined with MFr runoff  |
| MFdrain%r     | Effect of mitigation measures on tile drainage (relevant?)   | user input; probably not relevant  |
| MFr runoff%r  | Effect of mitigation measures on run-off   | user input; changeable default (adapted from mitigation review)                          |
| MFdrift%r     | Effect of mitigation measures on spray drift   | user input, changeable default (adapted from mitigation review)                          |
| MFleach%r     | Effect of mitigation measures on leaching (relevant?)  | user input; probably not relevant  |
| UnitArear     | Area of a mapping unit (grid cell, cone sector), map   | to be constructed  |
| Slope         | derived from HYDRO-1k elevation data (resolution 1 km)   | can be replaced with finer resolved data (e.g. SRTM-derived slopes with 90 m resolution) |
| not named     | area-specific discharge (monthly mean discharge (MMQ) or Flow Duration Curves (FDC))   | GRDC in Koblenz, Germany   |

## 5.6 Communication and reporting of the results

Communication, reporting and mapping of results will be performed in Module 7. Within this module, a suite of decision rules will be used to interpret the calculated exposure distributions and identify appropriate mitigation and management activities. The module will facilitate to

- Display maps of dominant contamination pathways and also “raw” IDPR maps
- Display PEC maps (for each pathway), and change legend
- Aggregate modelling/meta-modelling results to obtain probabilistic PEC distributions on large scales (river basins, states) or to estimate spatial and temporal variability of pesticide losses
- Display figures (+ explanatory text) from the modelling (e.g. CDF)
- Display summary text (report).
- Display proposed mitigation strategies
- Export maps and reports in different formats.

Since there are considerable uncertainties in the output at the national and EU scale due to scarcity of information and limited resolution of spatial input data, the presentation of colour-coded schemes will in many cases be preferable to the presentation of numerical estimates. All presented results will be accompanied by a qualitative or quantitative estimate of uncertainty.

The recommendations of mitigation strategies will also include considerations how these mitigation strategies may influence contamination by other pollutants such as phosphate or nitrate. It is important to pursue integrated approaches to risk management rather than merely shifting the problem from one pollutant class to another.

Therefore, although FOOT-NES will not perform TER calculations or more sophisticated risk characterization itself, it will offer convenient facilities to export PEC maps or distributions. The exported exposure concentration distributions (ECD) can then subsequently be compared by the user outside FOOT-NES with species sensitivity distributions (SSD).

## 6 ADDITIONAL FACILITIES

### 6.1 Pesticide Properties Database

The performance and reliability of mathematical models is ultimately governed by the quality of the model input data. Whilst there are a wide range of sources for the type of input data that will be required by FOOT-NES not all are of the highest quality and a certain amount of experience and understanding of the science driving the model is required to choose the best data available. The FOOTPRINT PPDB seeks to solve this problem by bring the best sources together in a standardised electronic format. This database will be embedded into the FOOT-FS, FOOT-CRS and FOOT-NES software packages in MS Access 2003 format with Access 2000 file structure to ensure compatibility with most potential users. The database will also be available online.

This database (FOOTPRINT PPDB) will be a comprehensive database of physicochemical and ecotoxicological data relating to pesticide active substances. As the pesticide fate models and meta-models within the FOOT-tools will use the data in the database it is important that the data are of the highest quality possible. The best sources of information currently available are the monographs produced as part of the EU 91/414/EEC review process. These documents will be the first choice for data but they are not available for all pesticides and so alternative sources of data will be used including national government resources, manufacturers, online databases and peer reviewed scientific publications.

Data sets will be cross-checked against each other as a means of ensuring data integrity. Where different sources of data have widely different values these will be validated by comparison with the original publications wherever possible. The database will be actively updated as additional information is identified and new and/or better data becomes available. Each data item will be 'tagged' with a code indicating the confidence the developers have in its quality. Confidence values will be in the range 5 (high) to 0 (low). A low value will not necessarily indicate that the data is incorrect but only that it can not or has not been validated. Confidence values will be based upon:

- The source of the data (e.g. EU dossier, manufacturer, other database or publication). Some existing data sets are no longer being maintained and updated. For example EU dossier data will acquire a confidence value of 5 where as estimated data may acquire a 0 or 1.
- The publication date of the data if known. Very old data may not have been determined using the same scientific procedures, standards and protocols used by the most recent investigations.
- Whether or not the data reference can be identified and used to cross check the data
- The match the data is to the desired parameter. For example the acute toxicity endpoint for fish required is the 96hr LC50 for Rainbow trout (*Oncorhynchus mykiss*) or Bluegill sunfish (*Lepomis macrochirus*). If an exact match can not be identified but data for a different species or a longer duration is available this will be used but the confidence score amended appropriately.
- A judgement on the fitness for purpose will also be made. For example dissipation data for European soils are preferred to those where conditions and soil types are very different.

The database will hold:

- General data describing the chemical such as its appearance, chemical structure and formula and in which EU States it is registered for use.
- Environmental fate data. For example the pesticide octanol-water partition coefficient (Log P), normalized sorption coefficient (Koc) and soil dissipation half-life (DT50).

- Ecotoxicological data. For example acute and chronic endpoint data for fish, aquatic invertebrates and aquatic plants.

## 6.2 Multi-lingual translations

As introduced in Section 3.2 the FOOT-NES software will be tri-lingual. This will be achieved using software development tools that handle the translation automatically at software run-time. However, to achieve this an electronic language dictionary is required. All strings used in the user-interface (including pesticide active substance common names) will be held in a MS Access database and referenced by an Identification Number (IN).

Against each Identification Number in the database the translations are held for each language. In the software development phase the Identification Number is held rather than the string itself. At run-time the Identification Number is automatically replaced by the appropriate string in the chosen language.

The following language translations are planned: English, French and German. The integrity of the translations is being addressed by ensuring that the translation is carried out by the appropriate FOOTPRINT partner i.e. a native language speaker also fluent in English. The responsible persons for the integrity of the language translations are Kathy Lewis (English), Olivier François (French) and Stefan Reichenberger (German).

## 6.3 User help and support facilities

User support facilities will be embedded into the FOOT-NES software at all operational levels. The types of help that will be available will include:

- Standard indexed help text and glossaries. This will comprise of written descriptions of both the operational and technical aspects of FOOT-NES.
- The User Manual in an electronic format will be available for browsing.
- Screen by screen support providing guidance on data entry and data requirements.

Help and support will be accessible to users via a variety of methods including:

- A separate FOOT-NES help menu in the ArcGIS menu bar
- All FOOT-NES data input and output screens will have Help buttons and Help icons. Help buttons will link users directly with specific Help text, bypassing the Help index. Help icons will be used to provide additional support such as explaining data input needs at a particular part of the software.
- Each part of the GUI's architecture (i.e. menus, data input boxes, buttons etc) will have associated 'tool-tips'. Tool-tips are used in conjunction with a cursor, usually a mouse pointer. The user hovers the cursor over an item, without clicking it, and a small box appears with the name or description of the item being hovered over.

# 7 EVALUATION, REFINING AND POLISHING PROCESSES

## 7.1 Evaluation

The reliability and usability of the FOOT-NES tool will be assessed through a substantial programme of bench and beta testing, and of evaluation studies of the tool's predictive capability.

Once the first draft of the software is completed a series of in-house bench testing exercises will identify and correct stability problems, obvious bugs and usability short-comings. The bench testing will, among other things, include:

- testing of FOOT-NES outputs against the standalone MACRO and PRZM meta-models,
- testing of drift calculation algorithms against the standalone equations to ensure that the implementation was error-free.

- testing of shell and database functionality
- testing of correct integration into ArcGIS

On completion of the bench testing a beta-version of the software will be available for testing by FOOTPRINT partners, AC members and any other interested persons.

The beta and final version of FOOT-NES will benefit from a substantial evaluation exercise where the predictive capability of the tool will be tested. At the national and EU scale, the only possibility of establishing confidence in the tool's predictive capability is to demonstrate that the tool can produce a statistical distribution of Predicted Environmental Concentrations (PEC's) that corresponds to measured data on exposure at the national level. Different approaches will be applied to predicted environmental concentrations for surface water and for groundwater because of the different exposure end-points used in the modelling approaches. For surface waters evaluation tests will be based on time-series of concentrations in 'edge of field' water bodies, whereas for groundwater, the validation focuses at the likelihood of contamination of the local groundwater. Evaluation tests will be carried out at different levels depending on the water resource under investigation. For surface waters, evaluation will be based on national and EU level predictions of exposure concentrations in edge-of-field water bodies associated with the range of agro-environmental scenarios present, compared to the measured concentrations collected at national and EU levels. In undertaking the comparisons, the likelihood that measured data will be mainly related to catchment-level exposure rather than edge-of field exposure and thus will not include the more extreme exposure concentrations will be taken into account. For groundwater the predicted frequency of exceeding concentrations of 0.1 µg L<sup>-1</sup> will be compared to the measured frequency of exceedence obtained from the national monitoring programmes.

A key component of the evaluation is the availability of good quality monitoring data at both national and EU-scales. Suitable data have been identified for Great Britain, Denmark, France, and Germany. The data combines comprehensive but temporally infrequent data from national water resource monitoring programmes with local data from a limited number of sites but with good temporal resolution.

## 7.2 Refinement and software polishing

Feed-back from the evaluation tests (section 7.1) will provide information on bugs, usability problems, system failures and possible problems with the representation of processes or quality of spatial input data. These will be corrected and the system refined. If performance bottlenecks (cf. section 7.3) are identified, the code will be refined accordingly to increase resource efficiency of the software.

## 7.3 System performance

Software performance testing can serve different purposes. It can demonstrate that the system meets performance and/or functionality criteria. It can compare two systems to find which performs or functions better. Or it can measure what parts of the system may cause the system to perform badly or fail. The earlier a performance defect is identified, the easier it is to correct. In all cases, it is often crucial for the test conditions to be similar to the expected actual end use.

Performance testing for FOOT-NES will be undertaken via in-house bench-testing and seek to achieve the following objectives:

- Verify input data collation time. Bench testing will identify typical data input times for users to - verify that this is acceptable and to provide user guidance.
- Verify the system capacity versus model run-time. For example, the system could theoretically be used to assess multiple applications of a given pesticide on a number of crops in a diverse catchment with a large number of agro-environmental scenarios. Performance testing will identify when the model run-time becomes unacceptable to end-users or when the data required or generated exceeds software or hardware capacity.

- Determine the optimal hardware/software configuration for FOOT-NES.

## 8 DOCUMENT MANAGEMENT

This document will be updated as soon it becomes necessary in the development process. Each new document version will supersede its precursor and be labelled with a version number and the date of creation (Table 9).

| <b>Date</b> | <b>Version</b> | <b>Description</b>                                       | <b>Authors</b>          |
|-------------|----------------|--|-------------------------|
| 30/12/2006  | 1.0            | First draft of FOOT-NES software specification document  | S Reichenberger, M Bach |
| 11/01/2007  | 1.1            | Second draft of FOOT-NES software specification document | S Reichenberger, M Bach |
| 27/02/2007  | 1.2            | Third draft of FOOT-NES software specification document  | S Reichenberger, M Bach |
|             |                |  |                         |

**Table 9: Revision history of this document**

## 9 GLOSSARY

### 9.1 Abbreviations, acronyms and proper names

| Abbreviation etc. | Description  |
|-------------------|--|
| CCM2              | Catchment Characterisation and Modelling Database v. 2   |
| CDE               | Convection-Dispersion Equation   |
| CDF               | Cumulative Distribution Function   |
| CLC2000           | CORINE Land Cover 2000   |
| CORINE            | Coordination of Information on the Environment   |
| CORPEN            | Committee of Orientation for Practices Respectful of the Environment. The CORPEN diagnostic methodology is widely used in France to characterise and mitigate the risk of pesticide transfers to groundwater and surface waters.   |
| DEM               | Digital Elevation Model  |
| DT50              | Dissipation half-life  |
| EU                | European Union   |
| FDC               | Flow Duration Curve = CDF of river discharge for a given time period (e.g. calendar month)   |
| FOCUS             | Forum for the Coordination of Pesticide Fate Models and their Use  |
| FOOT-CRS          | FOOTPRINT Catchment and Regional Scale Tool  |
| FOOT-FS           | FOOTPRINT Farm Scale Tool  |
| FOOT-NES          | FOOTPRINT National and EU Scale Tool   |
| FOOTPRINT         | Functional Tools for Pesticide Risk Assessment and Management  |
| GIS               | Geographic Information System  |
| GRDC              | Global Runoff Data Center  |
| GTOPO30           | a global DEM by USGS (United States Geological Survey) with a horizontal grid spacing of 30 arc seconds (ca. 1 km)   |
| GUI               | Graphical User Interface   |
| HOST              | Hydrology of Soil Types.<br>A delineation of UK soil types according to their hydrological properties to produce the 29-class Hydrology of Soil Types (HOST) classification. It is available as a 1km × 1 km grid.   |
| HYDRO1K           | HYDRO1K is a geographic database developed to provide comprehensive and consistent global coverage of topographically derived data sets, including streams, drainage basins and ancillary layers derived from GTOPO30.   |
| IDPR              | French acronym for “Index of development and persistence of hydrological networks”. A methodology which yields the natural tendency of a given area to let water infiltrate or to transfer water to an adjacent surface water body.  |
| Koc               | sorption coefficient normalized to organic carbon content of the soil  |
| MACRO             | not an acronym; name relates to macropore flow.<br>MACRO is a physically-based one-dimensional numerical model of water flow and reactive solute transport in field soils. MACRO is able to simulate tile drain outflow, leaching via preferential and matrix flow, decay, plant uptake, and foliar washoff of pesticides. |
| MS                | Microsoft ®  |
| NUTS              | Nomenclature of Territorial Units for Statistics   |
| PDF               | portable document format   |
| PEC <sub>gw</sub> | Predicted Environmental Concentration in Groundwater   |
| PEC <sub>sw</sub> | Predicted Environmental Concentration in Surface Water   |
| PPDB              | FOOTPRINT Pesticide Properties Database  |



|       |  |
|-------|--|
| PRZM  | Pesticide Root Zone Model.<br>PRZM is a one-dimensional, dynamic, compartmental finite-difference model that can be used to simulate chemical movement in unsaturated soil systems within and immediately below the root zone. The PRZM model is able to simulate surface runoff, erosion, chromatographic leaching, decay, plant uptake, foliar washoff, and volatilisation of pesticides |
| SGDBE | Soil Geographical Database of Europe   |
| SMU   | Soil Mapping Unit  |
| SRTM  | Shuttle Radar Topography Mission.<br>The NASA Shuttle Radar Topographic Mission (SRTM) has provided digital elevation data (DEMs) for over 80% of the globe (60° N to 56° S). These data are currently distributed free of charge by USGS and are available for download. The SRTM data are available as 3 arc second (approx. 90m resolution) DEMs.                                       |
| STU   | Soil Typological Unit  |
| TER   | Toxicity/Exposure Ratio  |
| WFD   | Water Framework Directive, 2000/60/EC  |

## 9.2 Technical terms

| Technical term                        | Description  |
|---------------------------------------|--|
| bound residues                        | also: non-extractable residues (NER)<br>Bound residues represent compounds in soils, plants or animals which persist in the matrix in the form of the parent substance or its metabolite(s) <i>after extraction</i> . The extraction method must not substantially change the compounds themselves or the structure of the matrix. (Führ et al., 1998)   |
| catchment                             | A catchment (also called drainage basin or watershed) is a region of land where water from rain or snowmelt drains downhill into a body of water, such as a river, lake, dam, estuary, wetland, sea or ocean. The drainage basin includes both the streams and rivers that convey the water as well as the land surfaces from which water drains into those channels. Each catchment basin is separated topographically from adjacent catchments by a ridge, hill or mountain, which is known as a water divide. |
| dispersion                            | Dispersion is the process of solute mixing due to different travel lengths and travel times of molecules. Dispersion occurs in several media (e.g. in soils, rivers etc.) and at several scales. It increases with lateral scale and travel distance. Dispersion causes sharp solute fronts to blur, and solute breakthrough curves to broaden, flatten and develop a tail. The process of dispersion is not to be confused with molecular diffusion, which is driven by concentration gradients.                |
| FOOTPRINT agro-environmental scenario | unique combination of a FOOTPRINT soil scenario, climate scenario and climate-specific agronomic scenario  |
| meta-model                            | In the field of environmental modelling, “meta-model” means a quick-running emulator of a more complex numerical model. Often a meta-model is based on interpolation, regression or neural networks.   |
| mitigation                            | In the context of FOOTPRINT, this term is used in a broad sense synonymously to “risk reduction”. Hence, pesticide mitigation comprises all measures that lead to a lower risk to the environment or human beings due to pesticides. This would include also switching to another pesticide with more favourable physical/chemical or  |

|            |   |
|------------|---|
|            | ecotoxicological properties.  |
| projection | A map projection is any method used in cartography to represent the two-dimensional curved surface of the earth or other body on a plane. The term "projection" here refers to any function defined on the earth's surface and with values on the plane, and not necessarily a geometric projection. There are several different types of projections, e.g. cylindrical, conic and azimuthal projections. |

**10 REFERENCES**

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Reichenberger S., Bach M., Skitschak A. & Frede H.-G. (2006). State-of-the-art review on mitigation strategies and their effectiveness. Report DL#7 of the FP6 EU-funded FOOTPRINT project [www.eu-footprint.org], 76 p.