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FOOTPRINT

Functional Tools for Pesticide Risk Assessment and Management

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Dubus I.G., Reichenberger S., Allier D., Azimonti G., Bach M., Barriuso E., Bidoglio G., Blenkinsop S., Boulahya F., Bouraoui F., Burton A., Centofanti T., Cerdan O., Coquet Y., Feisel B., Fialkiewicz W., Fowler H., Galimberti F., Green A., Grizzetti B., Højberg A., Hollis J.M., Jarvis N.J., Kajewski I., Kjær J., Krasnicki S., Lewis K.A., Lindahl A., Lobnik F., Lolos P., Mardhel V., Moeys J., Mojon-Lumier F., Nolan B.T., Rasmussen P., Réal B., Šinkovec M., Stenemo F., Suhadolc M., Surdyk N., Tzilivakis J., Vaudour-Dupuis E., Vavoulidou-Theodorou E., Windhorst D. & Wurm M. (2009). FOOTPRINT – Functional tools for pesticide risk assessment and management. www.eu-footprint.org. Final report of the EU project FOOTPRINT (SSPI-CT-2005-022704), 221 p.

Executive summary for policy- and decision-makers

1. The FOOTPRINT project (*www.eu-footprint.org*) combined the expertise of **15 partners from 9 European countries** to develop **methodologies and tools** for **pesticide risk assessment and management.**

2. The tools can **support MS and EU policies** related to the protection of **water quality** (Water Framework Directive and its daughter directives, drinking water legislations) or **pesticide use** (Directive on the Sustainable Use of Pesticides).

3. The FOOTPRINT software tools are based on the **latest developments in research** yet they are **carefully designed** to facilitate their use by non-specialists.

4. The 3 FOOTPRINT software tools operate at different scales and address the needs of different **environmental and agricultural** user communities:

    - **National and EU policy- and decision-makers** (country and continental scales)

    - **Water quality managers** (catchment and regional scales)

    - **Extension advisers and farmers** (local, farm scale).

5. The tools are **consistent across scales** and are operational **across all Member States**.

6. The tools can be used to **identify those situations** (soil, climate, crop, pesticide used, period of application, etc.) which are likely to lead to a **contamination of groundwater and/or surface water.**

7. FOOTPRINT is a key contributor towards **a sustainable European agriculture**.

8. A **start-up company "FOOTWAYS"** (*www.footways.eu*) has been created to ensure that the FOOTPRINT science is disseminated and tools are **supported in the long term**.

Executive summary for EU citizens

The European Commission funded a research project called FOOTPRINT to develop methodologies and tools to assess the risk of pesticides impacting on the environment. The FOOTPRINT partners developed 3 software tools which can be used to evaluate the risk of transfer of pesticides to water resources for any location in Europe. The tools can be downloaded for free through the web site *www.eu-footprint.org*.

Extended executive summary

Aims and objectives

The long-term sustainability of EU water resources is considered to be under threat as a result of their contamination by pesticides. There is a general lack of tools which would allow pesticide stakeholders, from decision-makers to farmers, to evaluate the risks associated with the use of pesticides and to investigate ways to limit the environmental transfers of pesticides.

In this context, the European project FOOTPRINT (*www.eu-footprint.org*), which was co-funded by the European Commission, developed three pesticide risk assessment and management tools, for use by three distinct end-user communities at three different spatial scales: policy makers and registration authorities at the national/EU scale, water companies and local authorities at the catchment scale, and farmers and extension advisors at the farm scale.

The three FOOTPRINT tools share the same underlying science and provide an integrated solution to pesticide risk assessment and management in the EU. The tools allow users to: i) identify the dominant pathways and sources of pesticide contamination in the landscape, ii) estimate levels of pesticide concentrations in ground- and surface water, and iii) make assessments of how the implementation of mitigation strategies would reduce pesticide contamination.

The FOOTPRINT methodology

The FOOTPRINT methodology consists in i) developing a detailed agro-pedo-climatic characterisation of locations where pesticides are used in the EU ('agro-environmental scenarios'), ii) simulating the fate of reference pesticides in the various scenarios; and, iii) integrating the modelling results in easy-to-use software tools.

Defining agro-environmental scenarios

The FOOTPRINT project developed and applied a methodology for defining a large number of generic scenarios that characterise the complete spectrum of European agricultural environments: the FOOTPRINT agro-environmental scenarios. Each agro-environmental scenario represents a unique combination of those climates, agronomic practices and soil characteristics which determine the fate of agriculturally-applied pesticides within Europe. This was achieved through the use of pan-European datasets on soil, climate, cropping and land cover. This allowed us to characterize the diversity of European agricultural and environmental conditions with respect to those parameters which most influence the environmental fate of pesticides. The various pan-European datasets have been intersected, using GIS, to identify the full range of unique combinations of climate, soil and crop types that characterize European agriculture. The FOOTPRINT agro-environmental scenarios and their supporting information are used to identify dominant contamination pathways for pesticides across Europe, to underpin model parameterization and to enable the spatial processing of the pesticide losses simulated by two pesticide fate models, MACRO and PRZM.

It is emphasized that although the agro-environmental scenarios developed have primary relevance to pesticide fate, they are also likely to be relevant to other potential environmental pollutants applied as part of agricultural practices within Europe (e.g. nitrate, phosphorus) because most of the driving climatic, soil and cropping characteristics are similar.

Simulating the fate of pesticides

A consistent and complete set of parameter estimation routines was developed for the MACRO and PRZM pesticide fate models to enable EU-wide simulations of pesticide leaching and pesticide inputs into surface waters via drainage, lateral subsurface flow, surface runoff and erosion. The soil parameterisation was based on analytical data and profile descriptions for each FOOTPRINT soil type (FST). Crop parameters were set according to literature information and the local knowledge of FOOTPRINT partners.

The macropore flow model MACRO was used in FOOTPRINT to predict pesticide leaching to groundwater and to surface waters via subsurface drainage systems. Some soil physical and hydraulic parameters of MACRO were derived with specific parameter estimation algorithms (‘pedotransfer functions’). This presented a scientific breakthrough, especially for parameters controlling macropore flow.

The PRZM model was used to simulate water fluxes and pesticide transfers originating from surface run-off and erosion. The system developed for model parameterisation was compatible with the data which are available at the EU level and the data farmers and extension advisors can gather quickly and at reasonable cost at the local field and farm scales. Before employing PRZM in FOOTPRINT, a conceptual problem in the model was alleviated. PRZM uses the SCS Curve Number approach for the calculation of surface runoff. However, the SCS Curve Number Approach is meant to provide an assessment of the stream response to heavy rainfall events and thus implicitly includes all components of fast flow to surface water (including, where applicable, also drainflow). We discovered that the SCS Curve Number approach was inadequately implemented in PRZM and we therefore adjusted the USDA soil hydrologic groups (which determine frequency and magnitude of runoff events) so that they reflect surface runoff only.

The fate of ca. 100 theoretical compounds (i.e. Koc/DT50 combinations) for all soil/climate/crop combinations relevant for Europe and 12 different application months were simulated using the pesticide fate models MACRO (predictions of pesticide loss for leaching, drainage and lateral subsurface flow) and PRZM (predictions of pesticide loss for surface runoff and erosion). The simulation period was twenty years for both MACRO and PRZM simulations. Summary statistics of every simulation time series were stored in a large number of MS Access databases, which are included in the FOOTPRINT tools. For surface water, the model output variables stored in the modelling database are: daily pesticide losses (drainage, lateral subsurface flow, surface runoff, erosion), associated water volumes or eroded sediment yield, resp., and the associated month. While in the FOOT-CRS databases maximum daily losses for each simulation month are stored, the databases used by FOOT-NES and FOOT-FS contain 11 percentiles of the whole time series (corresponding to return periods between 10 days and 10 years).

Calculating Predicted Environmental Concentrations in water

The pesticide losses from treated fields predicted by the models MACRO and PRZM were converted into actual inputs into surface water and groundwater, taking into account possible risk reduction measures. Subsequently, Predicted Environmental Concentrations (PEC) were calculated for groundwater (PECgw) and surface water (PECsw). These concentrations can subsequently be compared to legal (e.g. the drinking water limit 0.1 µg/l) or ecotoxicological thresholds. In the three FOOTPRINT tools, pesticide concentrations in water resources are calculated from simulated pesticide inputs by diffuse sources (spray drift, surface runoff and erosion, lateral subsurface flow, and tile drainage for surface water; leaching for groundwater).

In FOOT-CRS, the calculation of pesticide inputs into surface water accounts for the surface water network. PECsw are calculated at the catchment outlet (i.e. for one point in space). In contrast, in FOOT-NES and FOOT-FS, hypothetical edge-of-field water bodies adapted from FOCUS are used. PECsw and PECsed (sed = sediment) are calculated for each agro-environmental scenario, and afterwards spatially aggregated for display as map or as spatial cumulative distribution function. PECsw are calculated separately for each input path (surface runoff + erosion + interflow; drainage;

drift). FOOT-NES and FOOT-FS also allow the calculation of Predicted Environmental Concentrations in sediment (PECsed) and Time-Weighted Average Concentrations (TWACsw, TWACsed).

In FOOT-FS, the risk posed by a pesticide to the aquatic community is assessed by comparing predicted concentrations in surface water with the aquatic ecotoxicological endpoints for the taxonomic groups used as test organisms in the registration procedure (fish, invertebrates, sediment dwelling organisms, higher aquatic plants and algae) using the FOOTPRINT Pesticide Properties Database (PPDB), which is included in the FOOTPRINT tools. A simple toxicity/exposure ratio (TER) approach is used for this risk assessment; however, the user is able to view the PEC/TWAC calculated in FOOT-FS and use them to perform a more sophisticated ecological risk assessment (e.g., using mesocosm data or Species Sensitivity Distributions SSD) outside the FOOT tools. In FOOT-NES and FOOT-CRS, the user can obtain the (spatial or temporal, respectively) exceedance frequency of user-defined concentration thresholds from the PEC Cumulative Distribution Functions produced by the tools.

For groundwater, the same PEC calculation approach is used in all three tools. PECgw are calculated at a standard depth of 2 m. These predictions can then be combined with the FOOTPRINT SUGAR index (see below).

The three FOOTPRINT tools: FOOT-FS, FOOT-CRS and FOOT-NES

FOOT-FS (Farm/Field scale)

FOOT-FS has been developed for use at the local level (farm/field scale). The target users are agricultural advisers and farmers, although users can be anyone who wishes to explore crop protection scenarios at this level. The emphasis in FOOT-FS is on i) identifying the pathways and areas most contributing to contamination of local water resources by pesticides, and ii) providing site-specific recommendations to limit transfers of pesticides in the local agricultural landscape. FOOT-FS, which is available as a standalone application, automatically performs Toxicity/Exposure Ratio (TER) calculations for a range of aquatic taxonomic groups and for different temporal percentiles of exposure in a surface water body adjacent to the agricultural field of concern. The tool also suggests potential mitigation options allowing users to explore what-if scenarios and is supported with a number of tools and documents to help promote the adoption of good practices.

FOOT-CRS (Catchment and Regional Scale)

FOOT-CRS has been designed for scales ranging from small catchments to regional levels. The target users are water managers and include local authorities, environment agencies, water companies or stewardship managers. In FOOT-CRS, the emphasis is on i) identifying the areas most contributing to the contamination of water resources by pesticides, and ii) defining and/or optimising action plans at the scale of the catchment. FOOT-CRS uses the real surface water network. The tool uses the pesticide losses predicted by the pesticide fate models for each FOOTPRINT agro-environmental scenario and routes these through the landscape to the surface water network. For the calculation of pesticide inputs into surface water via surface runoff and erosion, a routing to the surface water network is performed using a Digital Elevation Model and the load reduction by reinfiltration or redeposition explicitly calculated. FOOT-CRS produces temporal distributions of concentrations in surface water at the catchment outlet (i.e. for one point in space), for different pesticide input pathways. These distributions can for instance be used to determine the return period of a given monthly maximum concentration for the pesticide of concern.

FOOT-NES (National and European Scale)

FOOT-NES has been designed for large-scale studies at national or EU level. The target users are EU/national policy and decision-makers of environment ministries and agencies. The emphasis in FOOT-NES is on i) identifying the areas most at risk from pesticide contamination and ii) assessing the probability of pesticide concentrations exceeding legal or ecotoxicological thresholds. Predicted Environmental Concentrations in surface water and sediment (PECsw and PECsed) are calculated for hypothetical edge-of-field water bodies. PECsw and PECsed are calculated for each agro-environmental scenario, and separately for each input path (surface runoff + erosion + interflow; drainage; drift). Finally, predicted concentrations for surface water and groundwater are spatially aggregated for display as map and for display as spatial cumulative distribution functions. The tool can be used to estimate the area percentage of exceedance of a given concentration in a region, a country or the whole of Europe.

Evaluation of the FOOTPRINT tools

Given the amount of time spent on the definition of agro-environmental scenarios, the modelling and tool development activities, only first-step validation activities of the tools were undertaken during the course of the FOOTPRINT project. The purpose of these activities was to evaluate the reliability and usability of the two tools.

Full beta testing of FOOT-FS and FOOT-NES in terms of bug detection and assessment of their operational efficiency were undertaken. The evaluations were performed using 'dummy simulation results' in those cases where there was a mismatch between timing for evaluation activities and the availability of modelling results for specific countries or regions. A fully functional beta version of the FOOT-CRS tool was not available in time for comprehensive testing due to the fact the partner responsible for its development resigned during the course of the project. Model evaluation activities are crucial for the credibility of any tool and the FOOTPRINT partners have engaged in an evaluation of the three tools on a voluntary basis beyond the end of the project.

Other outputs of FOOTPRINT

The FOOTPRINT PPDB

FOOTPRINT PPDB stands for FOOTPRINT Pesticide Properties DataBase. The database is used by all three FOOTPRINT tools as a source of active substances and their properties. The FOOTPRINT PPDB is a subset of the full PPDB managed and maintained by the University of Hertfordshire in the UK.

The objectives of the PPDB are to provide i) a single, comprehensive resource of reliable, consistently presented pesticide data; ii) a portable format for direct linking to software applications; and, iii) simple online access supported by layperson interpretations and user tools. The PPDB currently holds ~1000 records for active ingredients, plus 480 records for metabolites. The data include general information, physicochemical and environmental fate data, acute and chronic endpoints for a range of fauna and flora and information on human health issues. The database can be accessed through the FOOTPRINT web site *www.eu-footprint.org*.

FOOTPRINT SUGAR

FOOTPRINT SUGAR is a new hydrological index which can tell whether a particular area contributes more to groundwater recharge or to surface water discharge (SUGAR = SUrface water / GroundwAter contRibution). FOOTPRINT SUGAR was calculated for the whole of Europe and is available for free through the FOOTPRINT web site in the form of national datasets. FOOTPRINT SUGAR is based on the combination of two approaches for hydrological assessments: the hydrogeological IDPR index (which is computed using observed data only: a Digital Elevation Model (DEM) and an observed surface water network) and the SPR (Standard Percentage Runoff), which is used in catchment hydrology and which is available for each FOOTPRINT soil type.

Policy relevance

The preservation of the quality of water in the various Member States is of crucial importance for the long-term sustainability of natural resources. The FOOTPRINT methodology and tools can directly support two EU major initiatives:

The Directive on the Sustainable Use of Pesticides.

The Water Framework Directive and its daughter directives.

The tools can also have applications in pesticide registration pending modifications of the tools (see below and *www.footways.eu*) and in the context of the Cross Compliance of the Common Agricultural Policy.

Beyond FOOTPRINT

Long-term support for methodologies and tools beyond the end of the research funding is crucial if the science and associated software tools are to be used on a wide scale and in the long term. Numerous individuals and organisations which came in contact with FOOTPRINT have expressed their interest in using the FOOTPRINT tools, in benefiting from training and services and in commissioning new tools specific to e.g. one region or one crop.

As a direct follow up of FOOTPRINT, the project coordinator, Dr Igor Dubus, and a leading FOOTPRINT scientist, Dr Stefan Reichenberger, created a start-up company, FOOTWAYS, which provides services in the field of pesticide risk assessment and offers training and support in the use of the FOOTPRINT tools. For more information, please visit *www.footways.eu*.

Acknowledgements

The authors are grateful to the European Commission for the funding of the FOOTPRINT research project (EU contract SSPI-CT-2005-022704) under the 6th Framework Program for Research & Development. Sincere thanks are also expressed to members of the FOOTPRINT Advisory Committee who have significantly contributed to the success of the project. The reader's attention is drawn to the fact that the opinions expressed and conclusions drawn in this report are those of the authors, not necessarily those of the project's sponsor.

Project web site

The address of FOOTPRINT web site is: **www.eu-footprint.org**.

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CHAPTER 1 – INTRODUCTION

In view of the world's steadily growing population and demand of food and of severe global environmental problems at the same time, there is an increasing need for an environmentally sustainable agriculture. An important part of sustainable agriculture is to limit the risk to ground- and surface water resources posed by the use of crop protection products, i.e. pesticides. Several new pieces of EU legislation have been created in the last decade to move towards sustainable agriculture in Europe, notably the Water Framework Directive, the Thematic Strategy on the Sustainable Use of Pesticides with the new Framework Directive on the Sustainable Use of Pesticides and the revision of the registration Directive 91/414/EEC.
To ensure sustainability of agriculture with respect to pesticide use, pesticide risk assessment and management do not only have to take place in EU and national registration procedures, but also at the catchment scale (WFD context) and the farm scale (Sustainable Use context).
However, there is clearly a gap between available pesticide risk assessment procedures and the needs of all stakeholders dealing with pesticide matters on the ground.

The adoption of council directive 91/414/EEC concerning the placement of plant protection products on the market represented a major breakthrough in pesticide risk assessment in the EU. The directive called for harmonised approaches to risk assessment for pesticide registration among member states in the EU, in which model calculations of exposure in various environmental compartments (e.g. surface water, groundwater) would play a central role. This approach replaced earlier risk assessment methodologies in common use in member states, based on laboratory measurements of persistence, mobility, ecotoxicity etc., expert judgement and various 'rules of thumb'. It soon became apparent that the implementation of 91/414 within the EU required the adoption of consensus methods for model-based risk assessment, which at that time did not exist. Therefore, a series of FOCUS (FOrum for the Coordination of pesticide fate models and their USe) working groups were set up to address this problem. At the beginning of this decade, the FOCUS Groundwater (FOCUS, 2000) and Surface Water (FOCUS, 2001) working groups have delivered consensus modelling tools and procedures that are applied to representative 'worst-case' agro-environmental scenarios, as a basis for risk assessment and authorisation at the EU level, for example, for groundwater and surface water (via input routes such as subsurface drainage, spray drift, and surface runoff and erosion). Similar tools and procedures are being used by some member states for authorisation of product uses.

Although the FOCUS groundwater and surface water scenarios constituted a major progress at the time of their creation, there are still some weaknesses and limitations in the tools and procedures that have been developed. For example, some key processes that are known to be important controls on pesticide fate and mobility in soils (e.g. preferential flow) are not or not sufficiently included in the models currently used for risk assessment. For instance, only one of the nine FOCUS groundwater scenarios has been parameterized for the preferential flow model MACRO. However, while pesticide displacement by preferential flow was traditionally considered an issue restricted to heavy clay soils, there is widespread evidence meanwhile that it also plays an important role in lighter textured loamy or silty soils, and that preferential flow in soils is the rule rather than the exception.

Apart from this failure to account for this important process, another perceived weakness in the FOCUS methodology is that the selection of scenarios was based on expert judgement, since the resources or data required to carry out a rigorous analysis to identify representative worst-case situations in the EU were not available. The extent to which these scenarios really meet the objectives that were set up has therefore not been properly quantified. In other words, the representativity of the FOCUS scenarios for the wide range of European agro-environmental conditions is subject to question. Although the FOCUS scenarios represent a useful first attempt to define harmonised first steps for active substance evaluation in the EU, 'higher tier' regulatory approaches that can account for the tremendous variation in agro-ecosystem characteristics at larger scales (i.e. catchment, regional, national and EU) are still lacking. Some first attempts at spatially-distributed higher-tier risk assessments for pesticide registration have been made, for example, the tiered procedure in the Netherlands based on the GeoPEARL model. However, GeoPEARL, which describes leaching as a chromatographic process, cannot deal with preferential flow and is thus inadequate for simulating pesticide losses in the ca. 40-50% of EU soils for which preferential flow is the main controlling factor with regard to pesticide losses.

The Water Framework Directive (WFD) represents another major milestone in water quality legislation, putting into place a consistent framework for monitoring and assessing the chemical and ecological status of surface waters and groundwater, and placing in the hands of water authorities, the responsibility for either maintaining or improving water quality at the catchment or river basin scale. In this context, catchment-scale monitoring and experimentation have clearly demonstrated that 'point sources' (spills and accidents during filling and cleaning of equipment) contribute significantly to surface water contamination by pesticides. The term 'diffuse pollution', used to describe losses arising from normal agricultural use, may also be misleading. Indeed, recent research shows that, in reality, 'diffuse pollution' comprises a number of leaching or runoff 'hot spots' in the landscape, sometimes also referred to as "critical source areas". This is not surprising given the large variation in agro-environmental conditions and landscape attributes usually found within even small areas. In the context of the WFD, this implies that the development of expert systems and modelling tools that would allow policy-makers and water managers to identify the main sources and pathways (both point

and 'diffuse') of pesticide contamination at the catchment scale would be a cost-effective way to mitigate pesticide impacts on ground- and surface water.
This kind of user-friendly 'tailor-made' modelling tool is not yet available. Instead, empirical indices, such as the DRASTIC methodology, are often used to assess the vulnerability of water resources in the context of the WFD. These indices are based on a highly subjective combination of a range of environmental factors that are thought to control contaminant transport to surface water and groundwater. They are generic (i.e. they are not specific to pesticides) and cannot therefore distinguish between the huge variations in risk arising from a wide range of different compound properties and product uses. 'Attenuation factors' and other similar analytical equations have the advantage of accounting for compound properties, but the simplifying assumptions underlying their derivation (i.e. steady-state water flow) introduce serious errors into the predictions. Little use has so far been made of numerical simulation models for pesticide risk assessment at the catchment or regional scale, due to the complexity and variability of the soil-subsoil system, and the lack of data with which to parameterise the models. Similarly, little use has been made of process-based models in risk assessment for surface waters, as very few distributed rainfall-runoff models are adapted to handling pesticide transfer, and even if they are, the data requirements are usually prohibitive.

The Sustainable Use Directive aims to fill the current legislative gap regarding the use-phase of pesticides at EU level and to reduce risks to human health and the environment from registered agricultural pesticide uses. With the implementation of this Directive, on-farm risk assessment and management will become much more important and possibly mandatory for farmers. However, similarly to the catchment scale, process-based pesticide fate models have not yet been used for environmental risk assessment and management at the local scale (i.e. farm or field), again primarily due to the 'data gap'. So-called 'environmental indicators' are generally used instead. These tools consist of combinations of empirical indices, some based on 'expert judgement', that are designed to help farmers and extension advisers decide on best-management strategies and practices for revenue maximisation and/or environmental protection. They usually integrate components that describe the potential influence of mitigation strategies on reducing environmental risks at the scale of the farm. Interestingly, there have been very few attempts to combine process-oriented pesticide fate models with environmental indicators or indices, to benefit from their respective strengths. This leaves farmers and extension advisors in the largest part of Europe without a suitable computer tool for pesticide risk assessment and management.

The central idea and overall objective of FOOTPRINT was to develop tools which can be used by all relevant stakeholder groups to:

- identify the dominant pathways and sources of pesticide contamination in the agricultural landscape.

- estimate levels of pesticide concentrations transiting towards surface water and groundwater.
- make scientifically-based assessments of how the implementation of risk reduction strategies (e.g. no-spray zones, grassed buffer strips, hedges) is likely to reduce pesticide contamination of water resources.

We realised already from the beginning that one tool would not be able to meet the demands of all stakeholders, for the following reasons:

- The spatial scales and purposes of application differ widely among stakeholders (from EU scale to farm and field scale, from EU and national policy making to risk reduction for a real field or catchment);
- There are also different levels of data availability at the different scales (e.g., from 1:1,000,000 soil maps available at the EU level to theoretically perfect knowledge of soil and site characteristics for a given field);
- The intended user groups differ in their computer skills and knowledge regarding how to use models.

As a consequence, we decided to develop three different tools, tailored to their scales of application and their intended user groups. The main operational objective of the FOOTPRINT project was therefore

1) to develop a suite of three pesticide risk assessment and management tools, for use at three different scales by three different user communities:
    - policy- and decision-makers, ministries, and potentially pesticide registration authorities at the EU and national scale ('FOOT-NES')
    - ‘water quality’ managers (i.e. regional/local authorities, water agencies, water providers) at the catchment scale ('FOOT-CRS')
    - Farmers and extension advisers at the local, i.e. farm and field scale ('FOOT-FS')

The FOOTPRINT methodology which was conceived and deployed during the course of the project consisted in:

1) characterising agricultural locations where pesticides are used in the EU, in terms of soil, crop and climate, to come with the 'FOOTPRINT agro-environmental scenarios';
2) deploying state-of-the-art research models to simulate the fate of reference pesticides in those agro-environmental scenarios;
3) integrating the modelling results in the FOOTPRINT software tools.

The present report describes the work undertaken in the FOOTPRINT project. Chapter ***

More details can be found in the FOOTPRINT deliverables which were produced during the course of the project and which can be downloaded from the project web site. Additional details can also be obtained by contacting the former FOOTPRINT coordinator or the FOOTPRINT partners.

CHAPTER 2 – THE FOOTPRINT AGRO-ENVIRONMENTAL SCENARIOS

1 OVERVIEW

The overall objective of this component of the FOOTPRINT project was to develop and apply a methodology for defining a large number of generic scenarios that characterise the complete spectrum of European agricultural environments. Each scenario represents a unique combination of those climates, agronomic practices, soil characteristics and subsoil hydrological properties that determine the fate of agriculturally-applied pesticides within Europe. The work reported here describes how this has been achieved using pan-European datasets on soil, climate, cropping and land cover to characterize the diversity of European agricultural and environmental conditions with respect to those parameters that most influence the environmental fate of pesticides. Each pan-European dataset has been intersected, using GIS, to identify the full range of unique combinations of climate, soil and crop types that characterize European agriculture.

It is emphasized that although the agro-environmental scenarios developed have primary relevance to pesticide fate, they are also likely to be relevant to other potential environmental pollutants applied as part of agricultural practices within Europe (e.g. nitrate, phosphorus) because most of the driving climatic, soil and cropping characteristics are similar.

2 FOOTPRINT SOIL TYPES AND ASSOCIATED ATTRIBUTES

A key component of the scenarios is the grouping of European soils into a limited number of FOOTPRINT Soil Types (FSTs), based on their hydrological, textural and sorption potential characteristics, especially those that are used to parameterize the MACRO (Larsbo *et al*, 2005) and PRZM (Carsel *et al*, 1985) pesticide fate models used in FOOTPRINT. The main objectives were to characterize a limited number of soil types suitable for modelling the environmental fate of pesticides in Europe such that they represent the complete range of relevant pollutant transfer pathways from the soil surface to surface water bodies as well as the complete range of soil sorption potential relevant to ‘reactive’ pollutants.

2.1 The FST Hydrological Component

In order to meet the objectives, the FST hydrological component encompasses two sets of categories, both derived from an integration of the Hydrology Of Soil Types (HOST, (Boorman *et al.*, 1995; Schneider *et al.*, 2007) and French CORPEN systems (Groupe "diagnostic" du CORPEN, 1996). Firstly, a set of 15 FOOTPRINT hydrological groups, coded L to Z differentiated according to their permeability, water regime and substrate hydrogeology. Descriptions of the 15 groups are given in Table 1 along with their significance for deriving hydrologic conditions for the MACRO and PRZM models.

FOOTPRINT hydrological code	HOST class	Description	MACRO bottom boundary condition	PRZM Soil Hydrologic Group
L	1, 2, 3, 5, 13	Permeable, free draining soils on permeable sandy, gravelly, chalk or limestone substrates with deep groundwater (below 2 m depth).	Unit hydraulic gradient	A
M	4	Permeable, free draining soils on hard but fissured substrates (including karst) with deep groundwater (below 2 m depth).	Unit hydraulic gradient	B
N	6	Permeable, free draining soils on permeable soft loamy or clayey substrates with deep groundwater (below 2m depth).	Unit hydraulic gradient	B-C
O	7	Permeable soils on sandy or gravelly substrates with intermediate groundwater (between 1 & 2 m depth)	Zero flow	A
P	8	Permeable soils on soft loamy or clayey substrates with intermediate groundwater (between 1 & 2 m depth)	Zero flow	B-C
Q	9, 10, 11	All soils with shallow groundwater (within 1m depth) and artificial drainage	Zero flow	A
R	17	Permeable, free draining soils with large storage, over hard impermeable substrates below 1 m depth	Zero flow	B
S	19	Permeable, free draining soils with moderate storage, over hard impermeable substrates at between 0.5 & 1 m depth	Zero flow	B-C
T	22	Shallow, permeable, free draining soils with small storage, over hard impermeable substrates within 0.5 m depth	Zero flow	C
U	20	Soils with slight seasonal waterlogging ('perched' water) over soft impermeable clay substrates	Zero flow	B-C
V	23, 25	Soils with prolonged seasonal waterlogging ('perched' water) over soft impermeable clay substrates	Zero flow	C
W	16	Free draining soils over slowly permeable substrates	Percolation rate regulated by water table height	B

FOOTPRINT hydrological code	HOST class	Description	MACRO bottom boundary condition	PRZM Soil Hydrologic Group
X	18	Slowly permeable sois with slight seasonal waterlogging ('perched' water) over slowly permeable substrates	Percolation rate regulated by water table height	B
Y	14, 21, 24	Slowly permeable soil with prolonged seasonal waterlogging ('perched' water) over slowly permeable substrates	Percolation rate regulated by water table height	B-C
Z	12, 15, 26, 27, 28, 29	All undrained peat or soils with peaty tops	Not modelled	D

Table 1 - Description of the hydrologic component of FOOTPRINT soil type codes and their relationship with hydrologic conditions for the MACRO and PRZM models.

Secondly, a suite of seasonally-differentiated conceptual models of contaminant flow pathways (Flow Pathway Categories, FPCs) for each of 7 HOST/CORPEN classes coded A to G. The FPCs differentiate soils according to their potential for rapid transfer of water from the land surface to the surface water network by various fast or intermediate rainfall/runoff response mechanisms. Descriptions of the 7 HOST/CORPEN classes are given in Table 2 along with their Standard Percentage Runoff (SPR) indices derived from the HOST system. These SPR indices show the difference in the magnitude of rainfall/runoff response associated with each class. An example of the suite of FPCs for HOST/CORPEN class A and their link with specific FOOTPRINT hydrological groups is shown in Figure 1.

HOST/CORPEN class	Description	SPR Index
A	Soils on impermeable substrates of such as massive, pre-quaternary clays or hard & non-porous rocks	30 - 60
B	Soils on slowly permeable substrates such as boulder clays, glacial till, marls or mudstones	20 - 45
C	Soils on permeable macroporous substrates such as loose sands, gravels or river terraces	10 - 35
D	Soils on permeable microporous substrates such as sandy or granular limestone, chalk or ‘clay with flints’, deep permeable loam or clay, or loose volcanic materials	2 - 10
E	Soils on moderately permeable microporous/fissured substrates such as non-karstic limestone or sandstone	10 - 20
F	Soils on impermeable but fissured substrates such as karstic limestone or volcanic rocks	20 - 30
G	Soils on recent alluvium or thick peat	20 - 35

Table 2 -Description of the seven HOST/CORPEN classes and their associated Standard Percentage Runoff Indices derived from the HOST system.

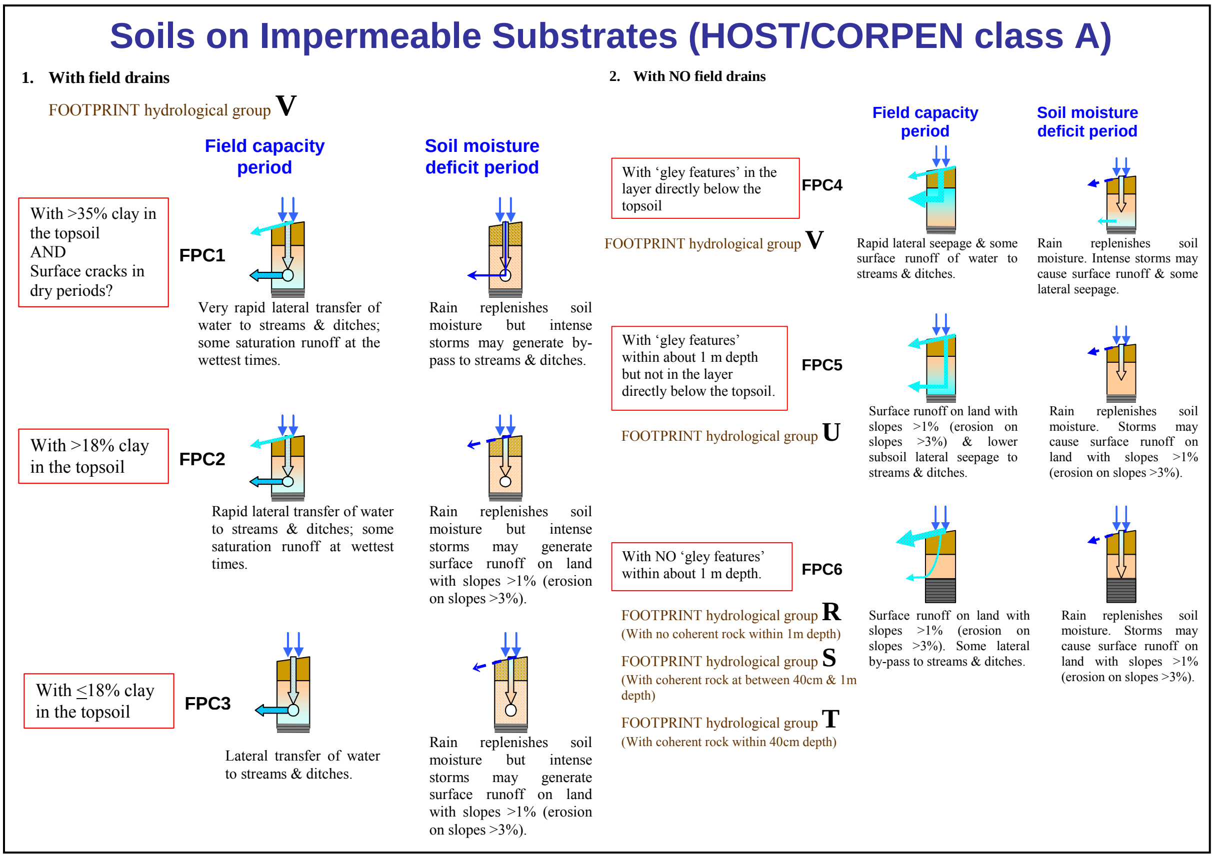


Figure 1 - Flow Pathway Categories (FPCs) for HOST/CORPEN class A soils and their associated FOOTPRINT hydrological groups.

2.2 The FST Textural Component

The textural component of FSTs uses the five textural groupings, coded 1 to 5, defined in the Soil Geographic Database of Europe (SGDBE, v.1) at 1:1,000,000 scale (Le Bas et al., 1998). The groupings are shown in Figure 2 and are used to characterise the upper part of the soil layer from 0 to 40 cm depth (the topsoil texture grouping) and the lower part of the soil layer from 40 to 100 cm depth (the subsoil texture grouping).

2.3 The FST Sorption Potential Component

Although clay type, soil pH and the presence of amorphous iron and aluminium oxides can all affect soil sorption of reactive compounds, for most organic compounds the principal sorption sites relate to soil organic matter. For this reason, most pesticide fate models require a compound-specific soil partition coefficient corrected for organic carbon content, the Koc in soil, as an input parameter. The final component of the FST thus allocates them to an 'organic profile class' based on broad differences in the magnitude and distribution pattern of organic matter within the soil profile. This attribute can be inferred from pedologically-based soil classification systems such as those used by many national soil survey organizations or the Food and Agriculture Organization (FAO-Unesco, 1974; FAO, 1998). Table 3 gives descriptions of each organic profile code used and the FAO (1998) soil class that can be used to identify it.

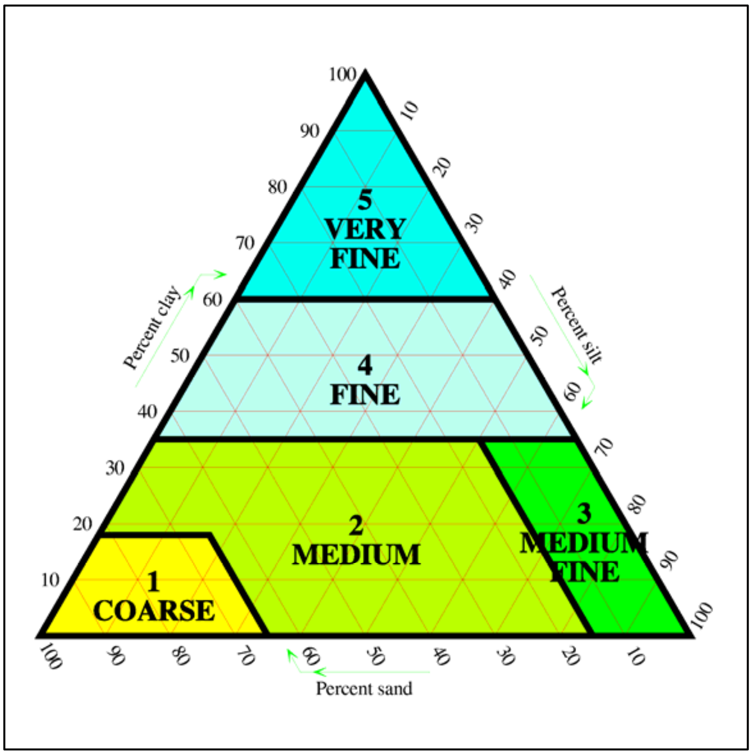


Figure 2 - -Groupings used to define the 'topsoil' and 'subsoil' textural components of FOOTPRINT Soil Types.

FOOTPRINT organic profile code	Description	SOIL (from SGDBE)
a	Alluvial soils with an uneven distribution of organic matter down the profile	Fluvisols, fluvic subgroups
g	With a thick (artificially deepened) topsoil relatively rich in organic matter	Plaggen soils
h	With an organic-rich topsoil	Chernozems, phaeozems humic & mollic subgroups
i	With a clay increase in the subsoil	Planosols, luvisols, podzoluvisols, luvic & planic subgroups
n	With a 'normal' organic profile	
f	Permafrost soils (non-agricultural) with an uneven distribution of organic matter down the profile	Gelic subgroups
o	Soils in volcanic material with organic-rich upper layers	Andosols
p	Podzols' with a relatively organic rich topsoil and an relatively organic rich subsoil layer	Podzols

FOOTPRINT organic profile code	Description	SOIL (from SGDBE)
r	Soils where the organic profile is limited by rock within 1 m depth	Rendzinas rankers and lithosols
t	With a peaty topsoil	Histosols & histic subgroups
u	Undeveloped' soils with relatively small organic matter content.	Regosols

Table 3 - Description of the 'organic profile' component of FOOTPRINT soil type codes and their derivation from the pedological SOIL code from the Soil Geographic Database of Europe (SGDBE).

An illustration of the differences in organic matter distribution within the soil profile for soils of the same hydrological and texture grouping but different organic profile codes is shown in Figure 3.

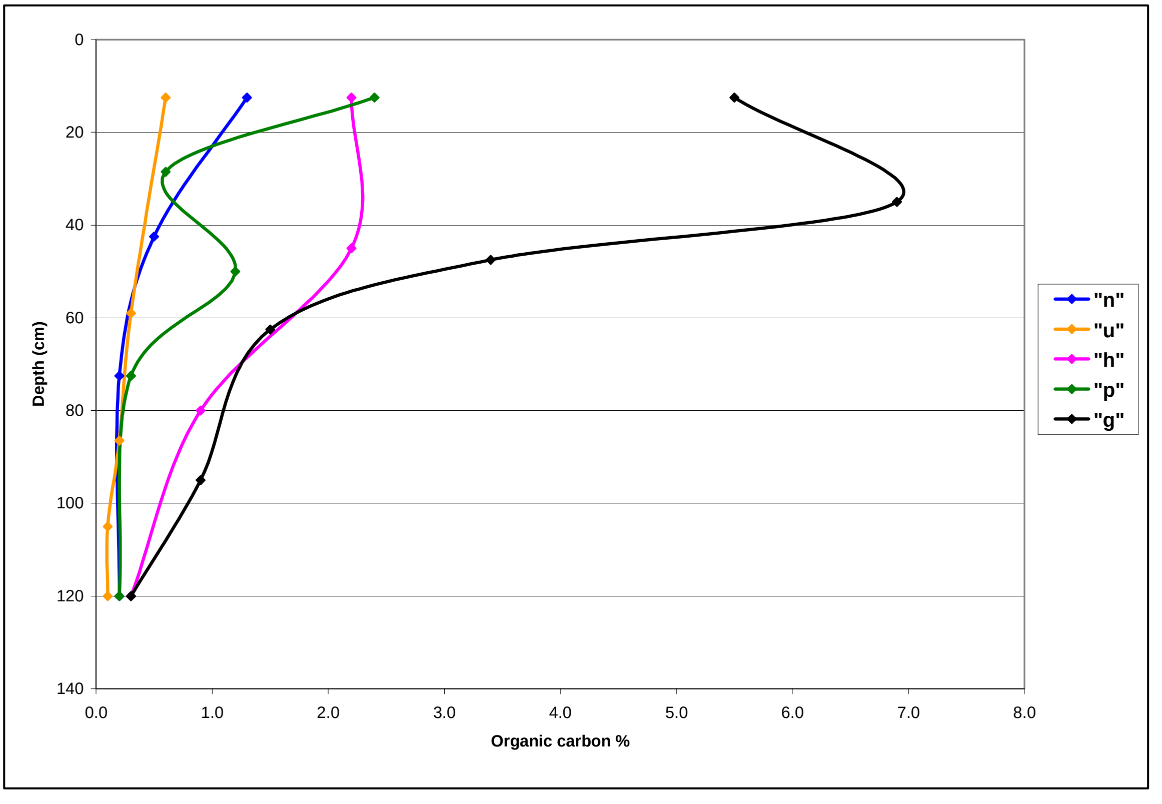


Figure 3 - Differences in the organic carbon profiles of soils with the same hydrological and textural grouping (L11) but with different FST organic profile classes.

2.4 The full FST code

The final FOOTPRINT Soil Type code was created by combining the codes for each of the hydrological, textural and organic profile components as shown in Figure 4.

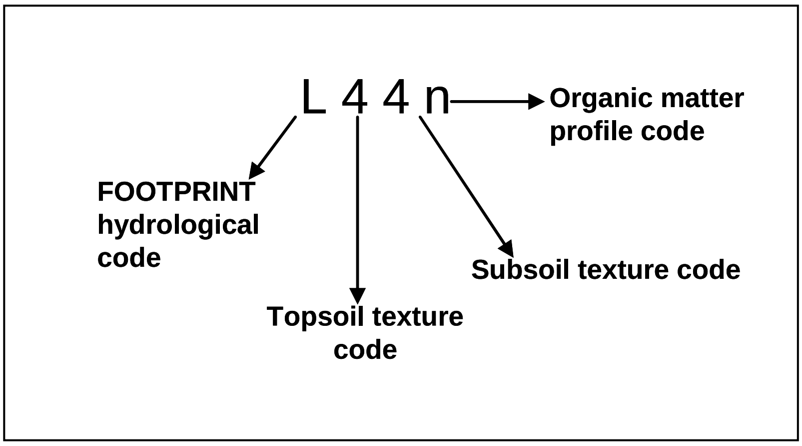


Figure 4 -The FOOTPRINT Soil Type code and its components

2.5 Identifying the range of FSTs within Europe

The Soil Geographic Database of Europe (SGDBE, v.1) at 1:1,000,000 scale (Le Bas et al., 1998) provides the only harmonized pan-European data that defines soil spatial variability. The database comprises polygon data files that define the location of Soil Map Units (SMUs), each of which comprises a number of defined Soil Types (STUs). The percentage cover of each STU within each SMU and some general attributes of each STU are defined in separate data files. It is assumed that this information represents the complete range of soil types within Europe and, using the attribute data, each STU in the SGDBE was therefore assigned to a FOOTPRINT soil type as follows:

- FOOTPRINT hydrological groupings were identified using the STU attribute data on FAO soil type code, soil parent material type, depth to obstacle to roots, water regime and water management system;
- Topsoil and subsoil textural groupings were identified directly from the TEXT1, TEXT2, TD1 and TD2 attributes of the STU attribute data file. However, where detailed particle-size data for an STU were available from the SPADE1 or SPADE2 databases (see section 2.6 below) this was used to check and, if necessary, adjust the texture codes;
- Organic profile classes were identified from the FAO soil class SOIL attribute using the relationships shown in Table 2.

This process resulted in 367 FOOTPRINT Soil Types (FSTs) representing all of the STUs in the SGDBE. Of these 271 represent soils under arable or permanent crops such as olives, fruit trees or vines, 297 represent soils under pasture (either intensively or extensively managed), of which 70 have pasture as the only agricultural use, and 18 represent soils that occur solely under non-agricultural uses.

2.6 Characterizing the properties of FSTs for modelling purposes

The SPADE1 and SPADE2 databases (Hollis *et al*., 2006), provide detailed profile-level data on soil properties for a wide range of European soil types within the SGDBE. Data on soil horizon type, depths, particle-size distribution, stone content, organic carbon content, pH and bulk density are available. Although the data do not cover all of the STUs in the SGDBE, there are still over 1,000 complete profiles with an agricultural land use available. Using these data, all arable or permanent crop (excluding pasture) soil profile data available for STUs with the same FST code were amalgamated and mean values for each parameter in each similar soil horizon calculated. This process provided data for most of the FSTs identified as having an arable or permanent crop land use, but some did not have any representative in the SPADE1 or SPADE2 databases. In such cases, synthetic land use specific property data were derived using the three components of the FST code. Thus, soil horizon sequences were derived from those FSTs with data that had the same hydrological class as the uncharacterized soil type. Particle-size data were derived from those FSTs with data that had the same topsoil and subsoil textural codes. Stone content, pH and organic carbon content were derived from those FSTs with data that had the same 'SOIL' and 'organic profile' codes as the uncharacterized soil type. Finally, bulk density was derived using a set of pedo-transfer functions incorporating particle-size distribution, organic carbon content and soil horizon type.

3 THE FOOTPRINT CLIMATIC SCENARIOS

A sensitivity analysis using the preferential flow model MACRO (Larsbo *et al*, 2005) was used to identify the critical climatic factors that influence pesticide fate by leaching and drainage (Nolan *et al.*, 2008). Univariate and multivariate statistics were used to relate predicted pesticide losses to climatic characteristics and 8 key climatic variables influencing pesticide fate were selected on the basis of these analyses. The 8 key climatic variables are: mean April to June temperature (ºC); mean September to November temperature (ºC); mean October to March precipitation (mm); mean annual precipitation (mm); number of days (April to June) where total precipitation >2 mm; number of days (April to June) where total precipitation >20 mm; number of days (April to June) where total precipitation >50 mm; number of days (September to November) where total precipitation >20 mm. A climatic classification for Europe was then constructed on the basis of these 8 key variables

(Blenkinsop *et al*., 2008). Within Europe, each variable was characterized spatially using two data sources: a) CRU TS 2.0 data set (Mitchell *et al*., 2004), and b) European Climate Assessment & Dataset (ECA&D) (Klein Tank *et al*, 2002). The analysis was based on data over the period 1961-1990. In order to take into account the likely correlation between several of the input variables, a dimension reduction procedure was performed using principal component analysis which resulted in the retention of 3 factors. These factors were then used as variables in a cluster analysis (k-means) which objectively grouped grid cells with similar characteristics. The final solution produced 16 groups (the FOOTPRINT climatic zones or FCZs) which represent a pragmatic compromise between producing a detailed classification and the need for a manageable number of representative climatic datasets for subsequent modelling work. A brief description of each climate zone and a summary of the EC Member States include in each zone is given in Table 4.

The spatial distribution of the 16 FCZs was digitized to provide a polygon dataset for GIS operations (Figure 5).

FOOTPRINT climatic zone (FCZ)	Description	Member States
1.Sub-mediterranean	Warm and moderate precipitation	France, Germany, Italy, Slovenia, Spain
2. Temperate maritime-influenced	Warm with moderate precipitation	Belgium, Denmark, France, Germany, Latvia, Lithuania, Luxembourg, Netherland, Poland, Sweden ,United Kingdom
3. Pre-alpine continental	Warm, moderate rainfall but low winter rainfall. More frequent spring extremes than other FCZ.	Austria, Czech Republic, Germany, Hungary, Italy, Slovenia
4. North European and continental	Cool and dry	Denmark, Estonia, Finland, Latvia, Lithuania, Poland, Sweden
5. Continental 3	Most warm and dry of the three continental climates	Not in the European Union
6. Alpine	Cool and wet. More frequent extreme spring rainfall relative to most FCZ.	Austria, France, Germany, Italy, Slovenia
7. Modified upland temperate maritime	Relatively high frequency of autumn extremes, but less than FCZ12 and relatively more frequent spring extremes than most FCZ.	United Kingdom
8. Mediterranean 1	Warmer and drier than FCZ1, but with similarly frequent extreme rainfall in autumn.	France, Greece, Italy, Malta, Spain
9. Mediterranean 2	Warmer, lower rainfall with more dry days but higher winter rainfall than FCZ8	Greece, Italy, Portugal, Spain
10. North European	Cold and dry	Finland, Sweden
11. Modified temperate maritime 1	Warmer and wetter than FCZ 2 but fewer wet spring days than FCZ 7	France, Portugal, Spain, United Kingdom
12. Wet mountainous maritime	Very wet, high frequency of autumn extremes	United Kingdom
13. Wet maritime	On exposed western coasts. Relatively high frequency of autumn extremes, but less than FZC12.	Ireland, United Kingdom
14. Continental 1	Warm and dry with moderate frequency of extremes	Austria, Czech Republic, Germany, Hungary, Poland, Slovakia, Romania
15. Continental 2	Warm and dry with less frequent spring extremes than FCZ14	Czech Republic, Germany, Greece, Hungary, Poland, Slovakia
16. Modified temperate maritime 2	Cool with moderate precipitation	Ireland, Sweden, United Kingdom

Table 4 - Summary description of the 16 FOOTPRINT European climatic zones identified by the cluster analysis and indication of European member states where each climatic zone can be found.

To represent the weather variation in each climate zone, an objective methodological analysis (Blenkinsop *et al.*, 2008) was used to select an ECA & D station displaying ‘average characteristics’ in relation to other stations present in the FCZ. Data from this station or from an equivalent MARS grid (MARS, 2007) were then used to create a 26-year daily weather dataset of precipitation, mean, maximum and minimum temperature, potential evapotranspiration, wind speed and solar radiation. For FCZ 6 (the Alpine zone) this process gave a set of weather data that reflected the average weather time series for sites above the tree line. This represents a fairly extreme weather pattern that does not relate to agricultural activity. However, in Slovenia, some agricultural activities do occur in FCZ 6 and the climate of these agricultural areas is similar to that of agricultural land occupying larger river valleys in the Alps. As a result, an alternative daily weather time series for FCZ6 was identified that better represented the agricultural areas of this zone.

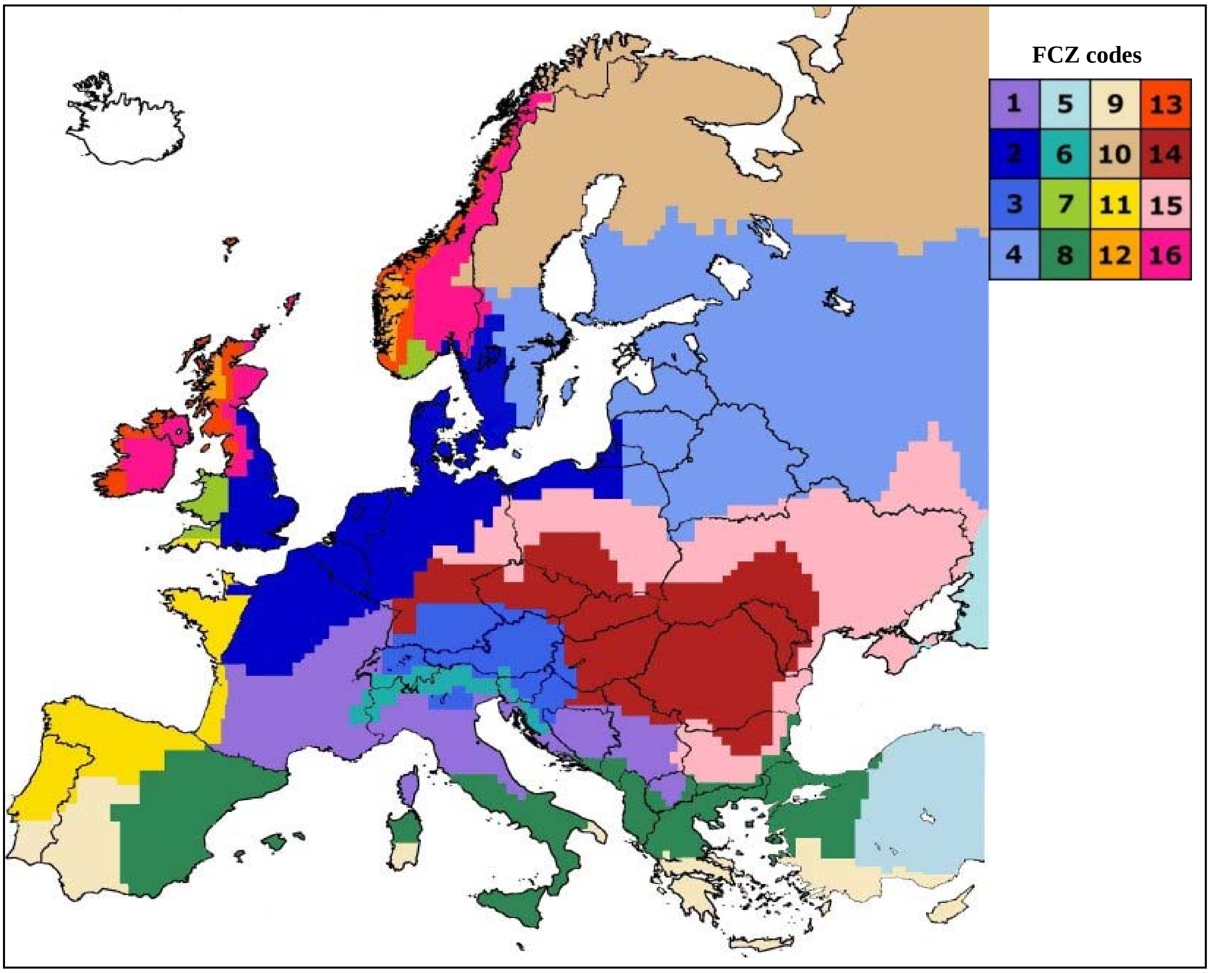


Figure 5 - Distribution of the 16 FOOTPRINT climate zones within Europe

4 FOOTPRINT AGRONOMIC CHARACTERISTICS

Agronomic scenarios are defined in this work as areas in Europe where the dates of specific crop growth stages and data on specific crop cover area and management practices associated with them, are similar.

The identification of such areas is based on the intersection of two datasets. The precise location of broadly different categories of agricultural land was defined using the CORINE (2000) Land Cover database at a spatial resolution of 250 m x 250 m. Only CORINE Land Cover (CLC) classes that represent agricultural land were selected to define agronomic scenarios and the following categories were used: Non-permanently irrigated (arable) land, permanently irrigated (arable) land, vineyards, fruit tree and berry plantations, olives, pasture, agro-forestry, annual crops associated with permanent crops, land principally occupied by agriculture with significant areas of natural vegetation and complex cultivation patterns. All other CORINE land cover categories were amalgamated as 'non-agricultural land' and not further differentiated.

In the resulting spatial database, whereas categories such as vineyards, olives, fruit trees and berry plantations and pasture represent land on which the agricultural crops are relatively permanent, categories that are characterized as partly or wholly arable represent land on which annual crops may vary from year to year. Within such categories therefore, the probability that a specific annual crop occurs at a certain location was determined using corrected European cropping statistics for the year 2000 from the FATE Land Cover map created by the JRC in Ispra (Grizzetti et al., 2007). The following crop categories or groups were included: barley, citrus, common wheat (= soft wheat) and spelt; cotton; durum wheat; fodder maize; fodderroot and brassica; fresh vegetables, melons, strawberries (outdoor); fruit and berry plantations; grain maize; greenfodder; hops; oats; olives; other cereals; other oilseed or fiber plants; permanent and temporary grass; potato; pulse; rape and turnip; rye; soya; sugar beet; sunflower; tobacco; vineyards.

To compute the shares covered by these crop groups for the FOOTPRINT agro-environmental scenarios, the FOOTPRINT default agro-environmental scenario shapefile (cf. Section 2.5) was overlaid with the FATE land cover map for the EU25 (100 m × 100 m grid) and the areas of the various FATE land cover types were tabulated for each of the 25044 FOOTPRINT agro-environmental scenario polygons, using the zonal statistics function "Tabulate areas" in ArcGIS. From the absolute crop areas and the polygon area, crop area fractions were computed for each polygon.

The procedure resulted in a fine resolution (≤ 250 m × 250 m) dataset that characterizes the spatial distribution of agricultural land within Europe and, for all agricultural areas, gives an estimated probability of occurrence of specific crop groups.

Finally, agronomic information, in the form of seasonal 'window' dates for sowing, germination, shooting, flowering and harvest, along with likely periods for pesticide application, was assigned to each crop in each NUTS level 2 (NUTS = Nomenclature of Territorial Units). This information was provided by FOOTPRINT project partners from various European countries who have access to local and national data on crop management practices. An example of such information is presented in Figure 6. Because these data incorporate different agronomic information for seasonal crop varieties such as autumn and spring sown barley or early and main crop potatoes, a total of 39 crop or crop varieties are included.

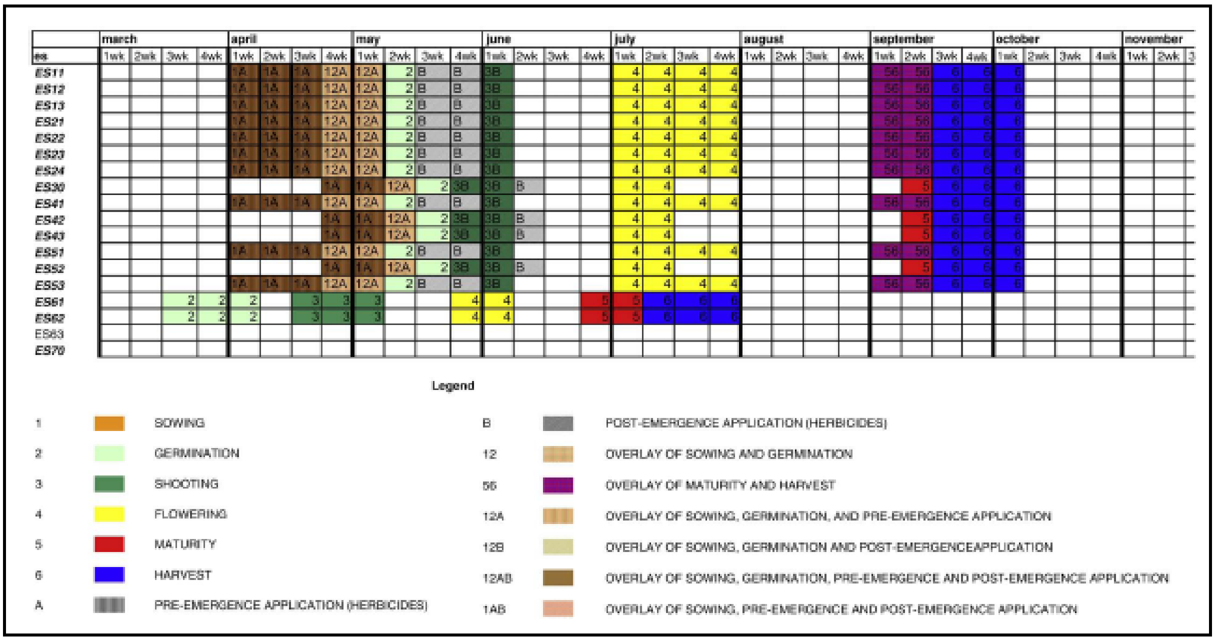


Figure 6 - Example of agronomic template of grain maize (spring sown) identifying seasonal 'window' dates for sowing, germination, shooting, flowering and harvest, along with likely periods for pesticide application for various NUTS level 2 in Spain.

5 CREATION OF THE FOOTPRINT AGRO-ENVIRONMENTAL SCENARIOS

Using a Geographic Information System (GIS; ESRI ArcGIS 9.1), the FOOTPRINT climate map, the CORINE Land Cover map and the NUTS level 2 map were intersected with the SGDBE shapefile (containing Soil Mapping Unit (SMU) polygons) to create the final FOOTPRINT default European agro-environmental scenario shapefile.

Because of the different resolution of the CORINE and SGDBE datasets, spatial inconsistencies were observed between those areas which, in the SGDBE (1:1,000,000 scale), are characterized as either 'undefined'; 'not surveyed'; 'soil disturbed by man'; 'water body'; 'glacier'; 'marsh'; or 'out of surveyed area' and equivalent areas in the CORINE data (250 m × 250 m). Where such areas had an attributed CORINE Land Cover class they were assigned to the Soil Map Unit of the nearest soil polygon rather than their original 'non-soil' designation from the SGDBE. This ensured that all areas identified as agricultural land by the fine-resolution CORINE data, had a designated soil type.

The final FOOTPRINT European agro-environmental dataset constitutes 25,044 multi-part polygon 'scenarios' (about 1.7 million individual polygons when converted to single-part polygons) derived by the intersection of the four spatial layers. Each polygon has a defined NUTS level 2 code, climate zone code, Soil Map Unit code and CORINE agricultural land code. Attribute data files linked to the spatial data define the fraction of arable crops related to each CORINE arable category as an indicator of its probability of occurrence, as described in section 2.2, and the fraction of each FOOTPRINT Soil Type in each Soil Map Unit, derived from the data held in the SGDBE. This fraction indicates the probability of occurrence of each FOOTPRINT Soil Type in each agro-environmental polygon.

Figure 7 gives a diagrammatic representation of the derivation and content of the European agro-environmental scenarios and an example of the GIS-based geographic representation of the scenarios is shown in Figure 8.

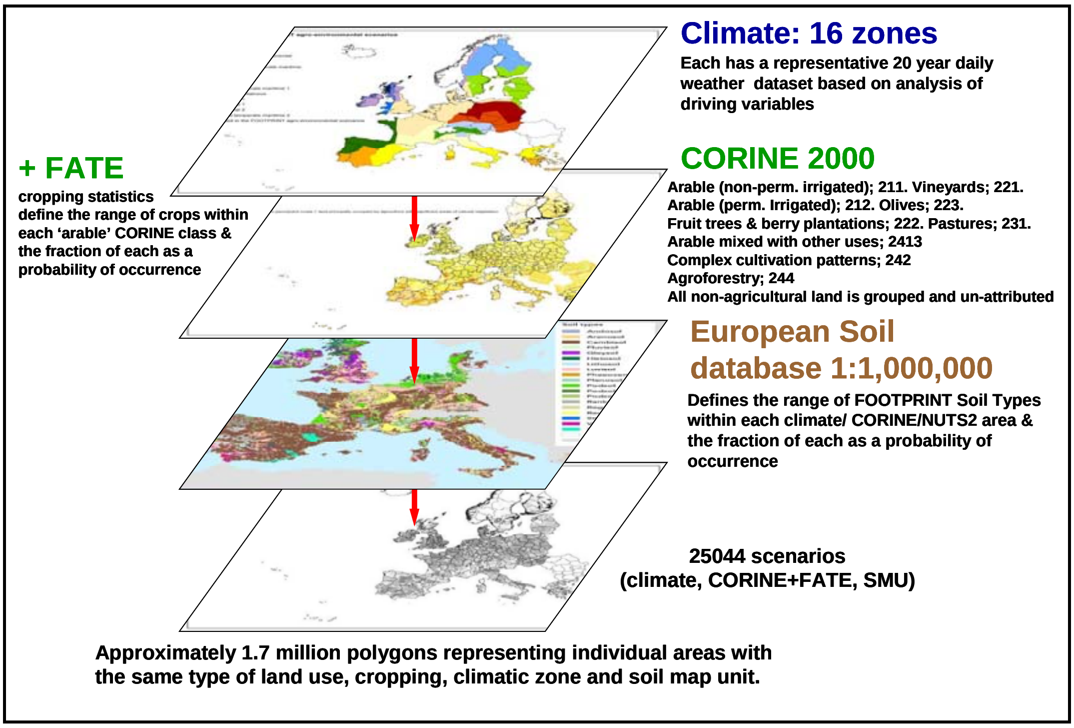


Figure 7 - Diagrammatic representation of the derivation and content of the European agro-environmental scenarios

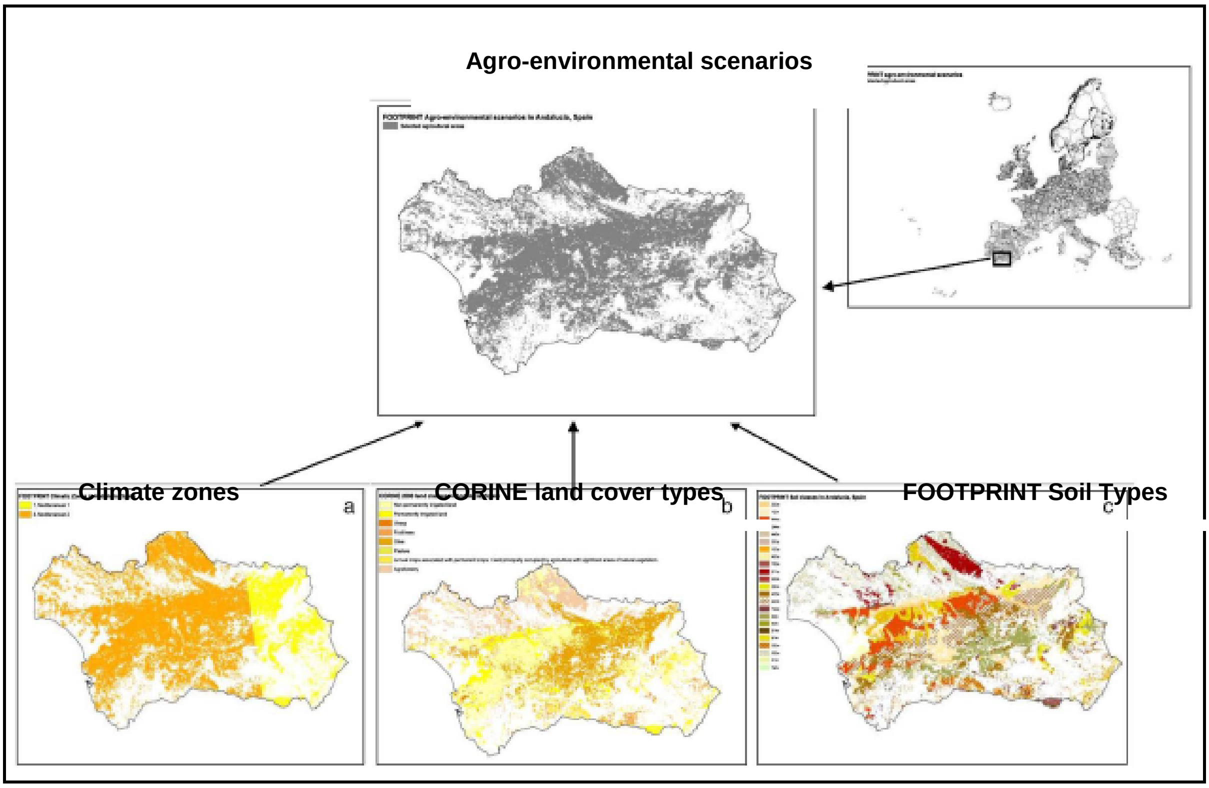


Figure 8 - Geographic representation of the FOOTPRINT agro-environmental scenarios using Andalucía as an example.

6 DISCUSSION AND PERSPECTIVES

A large number of agro-environmental scenarios representing land areas that are effectively homogeneous with respect to the critical factors controlling the environmental fate of agriculturally applied chemicals have been identified. Each unique combination of CORINE 'agricultural class', NUTS level 2 category, climate zone and Soil Map Unit (SMU) represents a single agro-environmental scenario in which the local soil is defined from a range of FOOTPRINT Soil Types with a defined percentage probability of occurrence and a defined range of annual and permanent crops with an estimated percentage probability of occurrence. A total of 25044 unique combinations of FOOTPRINT climatic zone, NUTS level 2, CORINE agricultural category and Soil Map Unit were identified. The 25044 scenarios represent the spatial variation and heterogeneity of the European agricultural landscape and, as far as we are aware, are the first attempt to quantify such variation at the pan-European scale. They can be used to underpin parameterization of pesticide fate models but, because most of the driving climatic, soil and cropping characteristics are similar, are also likely to be relevant to other potential environmental pollutants applied as part of agricultural practices within Europe (e.g. nitrate, phosphorus).

Further refinement of the approach could be based on incorporating more comprehensive and finer resolution data on crop and soil distributions as well as identifying locally representative weather datasets for individual soil and land combinations. In addition, integration of socio-economic aspects of farm structure could be used to refine the information on agronomic practices encompassed in the crop growth templates by indicating where differences in socio-economic factors may affect crop management techniques within areas with the same soil and climate.

6.1 Use of the scenarios for modelling the fate of agrochemicals within Europe

For modelling purposes it is only necessary to take into account the unique combinations of climate zone, soil type and crop that occur within Europe and when this is calculated from the agro-environmental scenario dataset, the total of unique combinations is 35158. This number takes into account the need for separate model simulation for autumn sown and spring sown varieties of the same crop, as well as early and late sown varieties of crops such as potatoes, soya, etc.

Each of the climate, FOOTPRINT soil type (FST) and crop components of the scenarios has an associated set of data which can be used to parameterize environmental fate models. Thus, each climate zone has a representative set of daily weather parameters for precipitation, mean, maximum and minimum temperature, potential evapotranspiration, wind speed, solar radiation for 20 years. Such a long period of daily data should be adequate to encompass most of the temporal variability in weather across the climate zone as well as including a sufficient number of extreme weather events to represent at least a 95^{th} percentile worst case for leaching, drainage or runoff. The crop calendar templates should also provide enough information to derive the crop growth input parameters necessary for modelling. Finally, the soil horizon type and depth, particle-size characteristics, organic carbon content, pH and bulk density data provided for each FOOTPRINT soil type can be used to derive any soil hydraulic characteristics required by models, using ‘pedo-transfer functions’ such as those included in the HYPRES database (Wösten *et al*, 1998) or derived from national datasets (Mayr & Jarvis, 1999). In addition, because the FST hydrological component identifies lower boundary conditions they have been used to derive some critical input parameters for MACRO. These, combined with a set of innovative decision trees for identifying soil susceptibility to macropore flow (Jarvis *et al.,* 2009) provide a state of the art basis for parameterizing the soil input data required by the model. Furthermore, the conceptual Flow Pathway Categories (FPC) associated with each FST (see section 2.1 of chapter 2) enable a surface runoff component to be separated from the ‘through-flow’ and drainage component of pesticide losses, thus facilitating an improved parameterization of the PRZM model for estimating surface runoff losses (Hollis, 2007).

6.2 Implication for improvement of risk assessment procedures

Current European risk assessment procedures use a limited number of scenarios to represent national and European spatial variability (a single scenario is used in the Netherlands, two scenarios are used in Denmark, and 10 scenarios have been defined at the EU level) (Van Alphen and Stoorvogel, 2002). In Germany Probst et al. (2006) and Herrchen et al. (1995) have identified eight different environmental scenarios in the central lowland region and five small scale national scenarios, respectively.

In contrast to these studies, the work presented here has derived a large number of agro-environmental scenarios representing land areas that are effectively homogeneous with respect to the critical factors that control the fate of agriculturally applied chemicals. The scenarios represent the spatial variation and heterogeneity of the European agricultural landscape and, because they incorporate data on the weather, soil physical, soil hydrological and crop growth characteristics that are required by most soil leaching, drainage and runoff models, they can be used to underpin their parameterization at the pan-European level. As such they provide a basis for developing a comprehensive probabilistic approach to estimating environmental exposure of agricultural applied chemicals within Europe. Probabilistic approaches to risk assessment for pesticides are currently under consideration (Hart, 2001), but a recognized limitation to such approaches is the lack of harmonised data at the pan-European scale, both for estimating exposure and effects. The agro-environmental datasets described here now provide the basis for addressing the exposure side of this problem.

At a more generic level, because the Flow Pathway Categories associated with each soil typological unit of the SGDBE differentiate land according to its different potential for rapid transfer of excess soil water to the surface water network, they allow a pollutant-specific set of effective mitigation strategies to be identified and associated with a specific soil component of each agro-environmental scenario. This process is illustrated in Figure 9 and has been incorporated into each FOOTPRINT tool to support a flexible approach to the management of pesticide environmental risks.

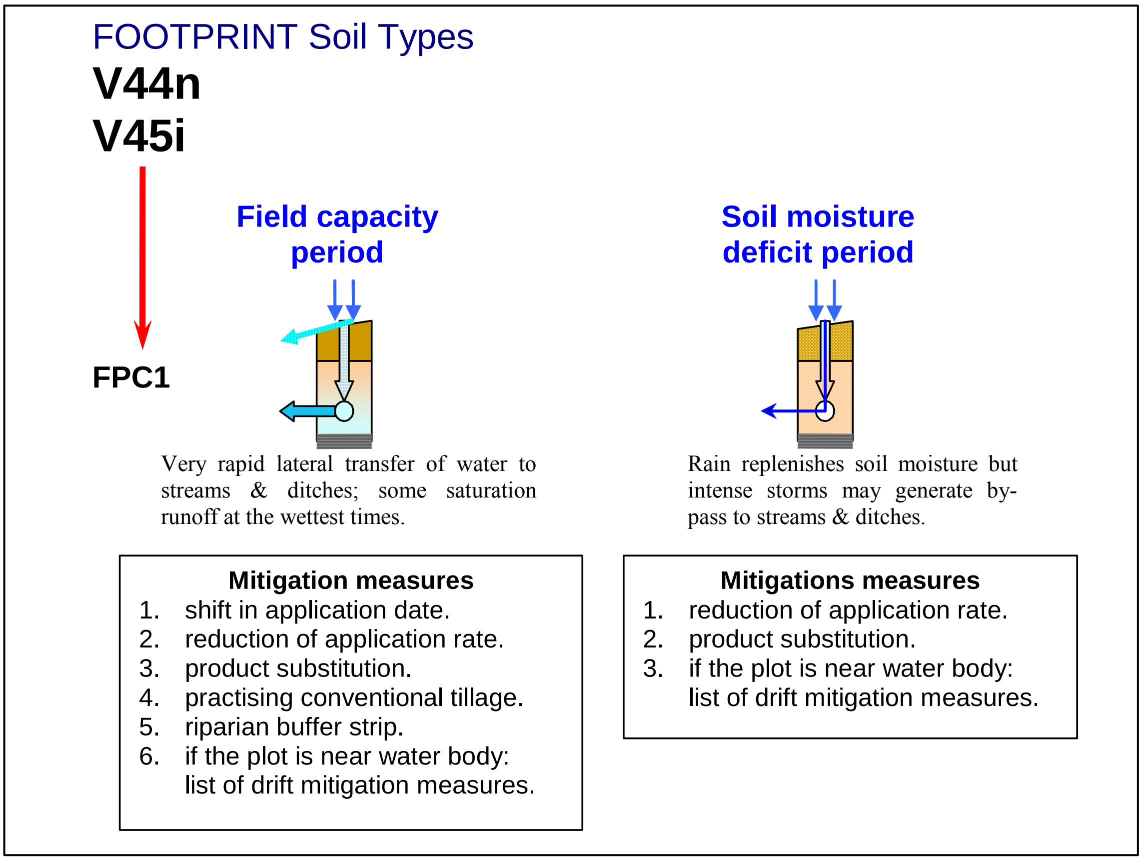


Figure 9 - Linking pesticide mitigation measures to a conceptual Flow Pathway Category (FPC).

6.3 Possibilities for further improvement of the scenarios

The agro-environmental scenarios described here have highlighted some variability in the complexity of scenarios between member states as well as shown the high spatial variability between small areas within the same country. The scenarios have the advantage of using harmonised pan-European datasets in their derivation but, at the regional scale, such an analysis can obviously be improved by incorporating more comprehensive or spatially precise data on weather, soil type and cropping, where it is available. When using such data to parameterize models, it is relatively easy to derive the required input parameters from local weather and cropping information. However, parameterization of soil and hydrological input requirements using local soil information is usually far less straightforward, not least because of the many different systems used to describe and classify local soil types within different European countries. In order to facilitate improvement of the scenarios by the incorporation of local and more detailed soil information, a comprehensive ‘decision-tree’ was developed to correlate local soil types with a FOOTPRINT soil type and its components soil hydrological and ‘organic profile’ information. The decision tree exists both in text form (as a set of MS-WORD files) and as a software module, the ‘FOOTPRINT Soil Selector’. Each consists of a series of questions relating to soil parent material, the presence of artificial drains, the presence of soil colours indicating intermittent waterlogging, organic-rich or organic-poor layers, topsoil and subsoil textures and the presence of coherent rock within 1-m depth. To help users make correct decisions, both tools include a comprehensive help text describing and defining the terms used. By using the decision tree scientists and practitioners can readily correlate a local soil type with a FOOTPRINT Soil Type and its associated soil parameter dataset for the MACRO and PRZM models. The identified FST can also be used to define the hydrological lower boundary condition and USDA Soil Conservation Service Soil Hydrological Group (see Table 1).

In addition the agro-environmental scenarios identified represent only one aspect of the variability of agricultural practices in respect to pesticide usage in Europe. Social aspects and economic factors also affect agricultural practices because individual farmer's managerial decisions are usually strongly influenced by local tradition, land inheritance, the national economy and global market forces.

For example, data on farm structure survey in 2003 (EC, 2005) show important differences between the structure of agriculture holdings among the 24 Member States. Most southern European countries are characterized by small holdings (5 to 20 ha) which rely heavily on family labour force and are often managed by farmers aged above 60 years. Such holdings have a small economic size and mainly focus on permanent crops such as vineyards, fruit, orchards, and olives. To a lesser extent, such socio-economic agricultural conditions extend into Slovenia and Hungary. In contrast, further north in Europe, a large proportion of holdings are more than 50 ha in size with at least about 4% being more than 100 ha. On average, holders are between 45 and 64 years old with Poland, Austria, Germany and Finland having 70% of holders aged less than 54. With the exception of Poland, the farm labour force on such farms comes mainly from outside the family and in many cases the holder has another profitable activity besides agriculture. The Netherlands, Denmark, Belgium, UK, and Czech Republic have the highest average economic size followed by Germany, France, Luxembourg, Sweden, Finland and Ireland. Lithuania, Latvia, Slovenia and Poland have the lowest average economic size, with economic production focussed solely on arable crops and grazing.

Such differences in socio-economic factors across Europe are likely to affect crop management techniques within areas with the same soil and climate and thus could be integrated with the biophysically-based scenarios described to develop sound and context-specific ecological risk assessment approaches.

CHAPTER 3 – PREDICTING THE FATE OF PESTICIDES IN THE FOOTPRINT AGRO-ENVIRONMENTAL SCENARIOS

1 OVERVIEW

This chapter presents the results of work carried out within the FOOTPRINT project to develop a consistent and complete set of parameter estimation routines for the MACRO (Larsbo and Jarvis, 2003) and PRZM (Carsel et al., 2003; FOCUS, 2001) models to enable EU-wide simulations of pesticide leaching and pesticide inputs into surface waters via drainage, lateral subsurface flow, surface runoff and erosion. The soil parameterisation is based on analytical data and profile descriptions for each FOOTPRINT soil type (FST, see Chapter 2). The following soil data, defined for each FST using the SPADE1 and SPADE2 databases, were used: FAO horizon designation; upper depth (cm); lower depth (cm); clay, silt and sand (%); stone content (%); pH; organic carbon content (%); bulk density (g cm^{-3}). Crop parameters were set according to literature information, especially FOCUS (2001) and the local knowledge of FOOTPRINT partners.

2 PARAMETERISING THE MACRO MODEL

The macropore flow model MACRO is used in FOOTPRINT to predict pesticide leaching to groundwater and to surface waters via subsurface drainage systems. Most parameters were not directly available, and therefore had to be derived from specific parameter estimation algorithms (‘pedotransfer functions’). This presented a considerable challenge, especially in developing algorithms to estimate the parameters controlling macropore flow. In this section, we describe the underlying hydropedological concepts and specific pedotransfer functions that have been developed in FOOTPRINT to estimate soil hydraulic functions and solute transport parameters, and the bottom boundary condition in the model, which largely controls the partitioning of excess water between groundwater recharge and discharge to surface waters. The crop parameterisation is also briefly described.

2.1 Soil hydraulic functions

2.1.1 Soil water retention

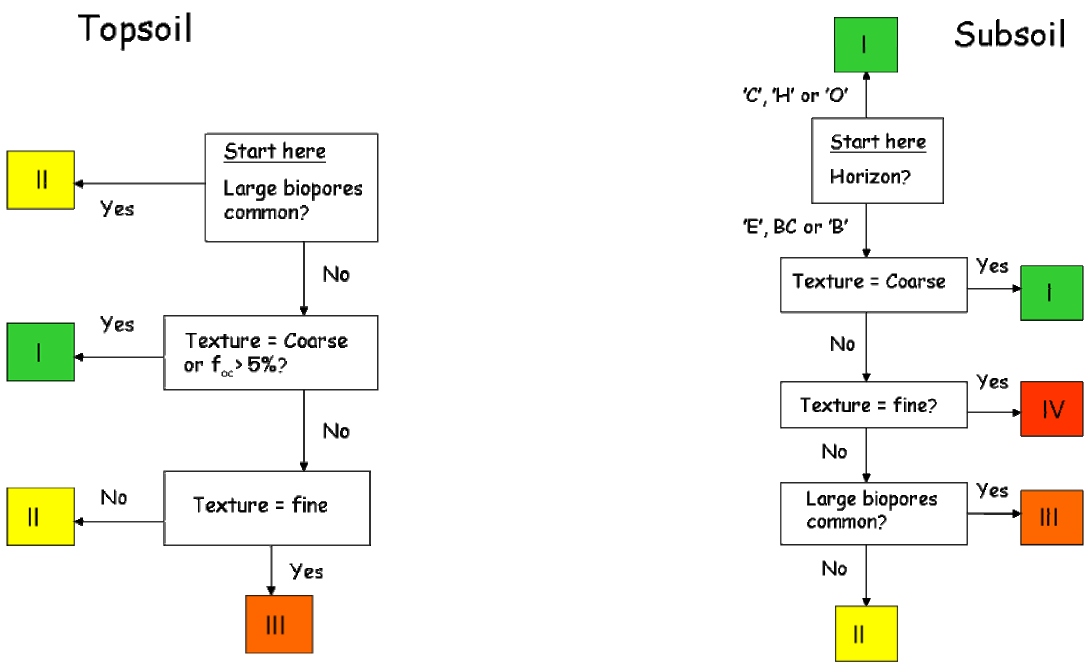
MACRO uses the van Genuchten (1980) water retention equation. The parameters of this soil water retention function (the shape parameters α, n, and the nominal saturated water content θ_s, assuming that m =1-1/n and the residual water content θ_r is zero) are estimated from basic soil properties (e.g. texture, bulk density, organic carbon content) using the HYPRES continuous pedotransfer functions (Wösten et al., 1999). Water retention parameters for organic horizons are set to fixed values (α = 0.013 cm^{-1} and n = 1.2) based on measured data for 148 organic soil horizons in Europe (Wösten et al., 1999). The nominal saturated water content θ_s predicted by HYPRES is corrected for stone content by multiplying by the factor $1-(f_s(1 - \varepsilon_s))$ where f_s is the stone content and ε_s is the stone porosity, which is assumed to be 0.1 for FOOTPRINT substrate geologies D, E and F (Chapter 2) and zero for all others.

In a review of the literature, Jarvis (2007) concluded that the weight of empirical evidence suggests that pores of ‘equivalent cylindrical diameter’ larger than about 0.3 mm can be considered as macropores. Thus, the minimum water potential defining the boundary between macropores and matrix in MACRO (parameter CTEN) is fixed at -10 cm, and the saturated matrix water content (i.e. XMPOR, the water content at -10 cm, θ_{10}) is estimated from the van Genuchten parameters. In this respect, it should be noted that the saturated water content θ_s calculated by HYPRES is only used to calculate the saturated matrix water content, θ_{10}, and is not actually used as a parameter in the model, since macroporosity (and thus total saturated water content) are estimated independently (see section 2.1.2 of chapter 3).

The wilting point water content (WILT) is estimated from the van Genuchten parameters as the water content at a tension of 150 m (pF 4.2).

2.1.2 Soil structure

Parameters controlling the strength of macropore flow in the model are estimated by class pedotransfer functions, since the experimental data were deemed insufficient to support the development of robust continuous functions. In our approach, a decision tree is used to place each horizon in the soil profile into one of four classes with respect to the potential for non-equilibrium flow in macropores (see Figure 10), ranging from ‘no potential’ (class I) to high potential (class IV). The decision tree was developed from a combination of quantitative analyses and expert judgement based on a literature review carried out within FOOTPRINT. The tree uses basic soil properties, land use, climate and management practices as input.



I = no potential, II = low potential, III = moderate potential, IV = high potential. Letters denote FAO (1990) horizon designations. Coarse texture = sand or loamy sand (USDA), fine texture = clay, silty clay or silty clay loam USDA). f_{oc} = organic carbon content.

Figure 10 -Decision-tree to classify soil horizons with respect to the strength of macropore flow.

The scheme shown in Figure 10 considers the influence of large biopores (defined as cylindrical pores >2 mm in diameter, equivalent to medium, coarse, and very coarse biopores according to FAO, 1990) on the potential for macropore flow. Permanent channels created by ‘anecic’ (deep-burrowing) earthworms are considered here as the dominant factor affecting macropore flow (large root channels are ignored). Several studies show a good correlation between the numbers of live earthworms, burrow numbers and hydraulic properties. There is considerably more literature on earthworm populations than burrow densities, especially for a few well-studied species like *Lumbricus terrestris* L. The biopore algorithm is therefore based on a literature meta-analysis of factors controlling population densities of *Lumbricus terrestris* (Lindahl et al., 2009) that includes measurements from 86 different sites in Europe. This simple algorithm correctly classified 79% of these studies.

Site factors			[d]Limiting soil texture
[a]Climate zone	[b]Hydrologic conditions	[c]Land use and management	
Cold temperate (FCZ 4,6,12,13,15)	All	Perennial	Coarse
Humid temperate (all other, except FCZ 10)	All	Perennial Annual	Coarse Coarse or fine
Mediterranean (FCZ 1,8,9)	Irrigated or FHC ≠ L,M or N	Perennial Annual	Coarse Coarse or fine

[a]FCZ = FOOTPRINT climate zone; [b]FHC = FOOTPRINT hydrologic class (see section 2.3); [c]Perennial = grassland, orchards, vines, olives; [d]Coarse = sand/loamy sand, fine = clay/silty clay/silty clay loam

Table 5 -Favourable site factors and soil textures limiting anecic earthworms.

Table 5 shows the combinations of site and soil factors that give favourable conditions for *Lumbricus terrestris*, defined as a population density greater than 8 individuals m^{-2} (c. 2 adult worms per m^2). Table 5 is combined with some simple rules to define one or more horizons in each FOOTPRINT soil type, that together comprise a zone in the soil profile which contains functional burrows, with respect to water flow and solute transport. The upper and lower limits, L_u and L_l, of the functional burrow zone are given by:

L_u = max(0, tillage depth)
L_l = upper boundary of first horizon with *limiting factor*

where *limiting factors* are one or more of the following: rock ('R'); drainage depth (see section 2.3.); 'BC', 'C' or 'O' horizon; pH<5; bulk density >1.75 g cm^{-3}; limiting texture (see Table 5).

Large functional biopores formed by anecic earthworms are then assumed to be common in a horizon (see Fig. 10) if:

(mid-point depth of horizon > L_u) and
(mid-point depth of horizon < L_l) and
(site conditions are potentially favourable, see table 1) and
(L_l minus L_u > 20 cm)

Two parameters in MACRO are directly estimated from the macropore flow classes (the effective diffusion pathlength ASCALE, and the kinematic exponent ZN, see Table 6) and one indirectly (saturated hydraulic conductivity, KSATMIN, see section 2.1.3 of this chapter).

Class	[a]Effective diffusion pathlength (mm)	Kinematic exponent
I	1	6
II	15	4
III	50	3
IV	150	2

[a]The effective diffusion pathlength is set to 3 mm in the uppermost intensively tilled layer in arable soil independent of class. Intensive tillage (e.g. harrowing, rotovating) shatters and pulverizes the soil to create a fine 'crumb' or granular structure, with a spherical geometry that maximises mass exchange

Table 6 -Class pedotransfer functions for soil structure-related parameters.

No suitable estimation routines were available to estimate soil macroporosity. Nevertheless, a review of the literature carried out within FOOTPRINT suggests that, as a structure-related parameter, macroporosity is closely related to observable horizon morphology and basic soil properties such as texture (Jarvis, 2007). Therefore, macroporosity is estimated as a function of the FAO (1990) horizon designation and the soil texture (see Table 7). The total porosity (TPORV) is then simply given by the sum of macroporosity and θ_{10}.

Soil	Horizon	[a]Texture		
		Fine	Medium	Coarse
Topsoil (mineral)	[b]Undisturbed	0.05		
	[c]'A_t'	0.05		
	[d]'A_p'	0.03	0.04	0.05
Subsoil (mineral)	[e]Upper 'B' or 'E'	0.016	0.016	0.05
	[f]Lower 'B' or 'E'	0.008	0.008	0.05
	'BC'	0.002	0.004	0.04
	'C'	0.002	0.004	0.03
Organic	'O'	0.05		

[a]fine=clay,silty clay,silty clay loam, coarse = sand, loamy sand, medium = all others; [b]perennial crops i.e. grassland, vines, orchards, olives; [c]intensively (secondary) tilled uppermost soil layer; [d]ploughed but not secondary tilled; [e]mid-point depth of horizon <50 cm; [f]mid-point depth of horizon >50 cm

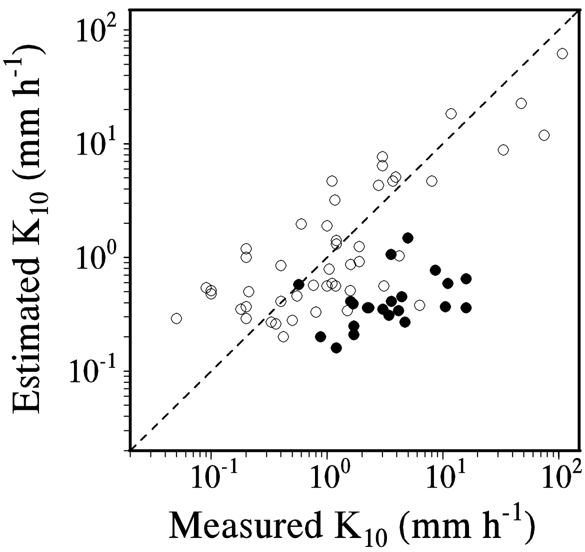
Table 7 -Class pedotransfer function for macroporosity.

2.1.3 Hydraulic conductivity

Jarvis et al. (2002) showed that hydraulic conductivity at -10 cm, K_{10} (KSM) measured by tension infiltrometer was reasonably well predicted by soil texture. However, a more physically-based approach predicting K_{10} from the pore size distribution (i.e. van Genuchten water retention parameters) would be preferable. From a strictly physical point of view, K_{10} should depend only on α and θ_{10} when m = 1-1/n and θ_r is zero (Mishra and Parker, 1990; Hoffman-Riem et al., 1999). We re-analysed the data in Jarvis et al., (2002) using this model, but the results were poor. This is presumably because the van Genuchten parameters were not available for this dataset, so they were predicted using the HYPRES pedotransfer functions. In particular, α is poorly estimated by the HYPRES function (Wösten et al., 1999). We therefore developed an empirical approach using n as a predictor variable (Wise et al., 1994):

$$K_{10} = C\theta_{10}n^{l} \quad (1)$$

where C and l are constants. Figure 11 compares measured and predicted K_{10} values with C = 0.186 mm h^{-1} and l = 10.73. The agreement is satisfactory, considering the errors involved in predicting n and in the measurement of K_{10}, not least because they were performed by ten different researchers (Jarvis et al., 2002). This is illustrated by the fact that the measurements from three of the researchers fall consistently below the 1:1 line (Figure 11). Considering how it was derived, equation (1) should only be used to predict K_{10} in conjunction with the HYPRES pedotransfer functions, and not from measured water retention data.



Data are taken from Jarvis et al. (2002), predicted values are calculated using equation 1, and θ_{10} and n are predicted by HYPRES. Solid symbols represent data obtained by three of the ten researchers.

Figure 11 - Measured and predicted saturated matrix hydraulic conductivity.

If it is assumed that the macropore size distribution follows a power law function (i.e. a water retention curve of the Brooks-Corey type) and flow is calculated according to a capillary bundle model based on Poiseuille's law with a fixed maximum pore size, then the macropore saturated conductivity $K_{s(ma)}$ can be expressed as (Jarvis, 2008):

$$K_{s(ma)} = \frac{B\varepsilon_{ma}}{n^*} \qquad (2)$$

where ε_{ma} is the macroporosity (see Table 7, n^* is the kinematic exponent (ZN, see Table 6) and B is a composite 'matching factor' accounting for both physical constants and the geometric irregularity of the functional macropore system, set here to 6000 mm h^{-1}. The total saturated hydraulic conductivity (KSATMIN) is simply given by $K_{10} + K_{s(ma)}$.

2.2 Rock hydraulic parameters

The FOOTPRINT hydrologic classes L, M and N represent free-draining soils overlying permeable rock, where recharge to groundwater is the dominant flow pathway (see Chapter 2). In some FOOTPRINT soil types the boundary between soil and rock occurs at relatively shallow depths (e.g. thin 'rendzina' soils overlying chalk or limestone). In these situations, MACRO must be run to a profile depth of 2 m (i.e. well into the rock layer) to ensure that a reasonable hydrology is simulated with the bottom boundary condition used (unit hydraulic gradient, see section 2.3 of chapter 3). This means that hydraulic properties must be defined for the permeable rock. Soil hydrologic groups L, M and N overlie substrate geologies D, E, and F, which mostly represent rocks such as fissured chalk, limestone and sandstone. For this special case of permeable rock horizons, we set the hydraulic parameters in MACRO to values that represent fissured limestone (Roulier et al., 2006), assuming a high potential for macropore flow (i.e. class IV): effective diffusion pathlength = 150 mm; $K_{s(ma)}$ = 30 mm h^{-1}; K_{10} = 0.04 mm h^{-1}; θ_s = 0.1 m^3 m^{-3}; α = 0.0004 cm^{-1}; n = 1.8; n^* = 2; ε_{ma} = 0.01 m^3 m^{-3}.

2.3 Site hydrology

Using the HOST methodology (Boorman et al., 1995), each FOOTPRINT soil type has been classified into one of 14 hydrologic classes (the FOOTPRINT Hydrological Groups (FHG); L to Y), on the basis of the major pathways of water flow and pesticide loss in the profile. The FOOTPRINT Hydrological Groups then form the basis of the parameterisation of surface runoff in PRZM and also affect parameters controlling drainage and leaching in MACRO, specifically the bottom boundary condition and the dimensions of any drainage system present. For MACRO, the 14 classes can be telescoped further into 8 unique hydrologic parameterisations (see Table 8). Three major groupings are recognised: classes L, M and N represent soils with free drainage to deep-lying groundwater. A unit hydraulic gradient bottom boundary condition is used, no drains are present, all excess water is routed to groundwater, and only pesticide leaching is output from the model (Table 8). Another group (W, X and Y) represents soils with slowly permeable substrate, that allow both recharge to groundwater and discharge to surface waters (via subsurface drains and/or lateral subsurface flow). A water table is found within the profile depth, and the bottom boundary condition is given by a percolation rate defined as a linear function of the water table height. Only discharge to surface water is simulated for the third group of soils, which either have impermeable substrates (i.e. hard rock or impervious clay, classes R to V) or are located in low-lying areas in the landscape (O to Q). The bottom boundary condition is, thus, zero flow and discharge is calculated as the outflow of subsurface drains or as lateral subsurface flow (which is in fact simulated in MACRO *via* an 'effective' subsurface drain system).

An effective drainage spacing, *L* (SPACE), is calculated for each soil type belonging to one of the FOOTPRINT hydrological classes which include discharge to surface water (classes O to Y), following the methodology introduced by Hooghoudt (1940):

$$L = \sqrt{\frac{8K_2 dh + 4K_1 h^2}{q_{eff}}} \tag{3}$$

$$d = \frac{D}{\left(\frac{8D}{\pi L}\right)\ln\left(\frac{D}{u}\right) + 1} \tag{4}$$

where d is a reduced 'effective' soil depth below the drainage base, q_{eff} is a design discharge rate, h is the design height of the water table above the drainage base, D is the actual depth of soil between the drainage depth (DRAINDEP) and the bottom of the profile (see Table 8), K_1 and K_2 are the weighted average saturated hydraulic conductivities (KSATMIN) across the soil depths h and D respectively, and u is the wetted perimeter of the drainage channel. The wetted perimeter of the drainage channel, which is unknown, is fixed at 0.2 m, although it could in reality vary between c. 0.1 and 0.5 m depending on the type of drainage system.

It can be noted from equations 3 and 4 that *L* depends on *d* and *d* on *L*. The drain spacing *L* is therefore found iteratively when *D*>0. *L* is an 'effective' drainage spacing: some FOOTPRINT hydrologic classes typically have field drains installed (e.g. parallel pipe or tile lines), while others would instead be drained by open ditches surrounding the field. Finally, in some classes (i.e. R, S, T, W and X), an 'effective' drainage system is simulated to mimic lateral downslope saturated flow above an impermeable substrate towards ditches and streams. In the absence of parallel field drains, the 'drain spacing', *L*, can be related to the effective area of a square-shaped drainage basin (Larsbo and Jarvis, 2003).

Hydrologic class	Drainage depth (m)	Depth of profile (m)	Bottom boundary condition	MACRO output variables
L,M,N	N/A	2	Unit hydraulic gradient	Percolation rate Leaching rate
O,P	2	2	Zero flow	Drainage rate Loss in drain Conc. at base
Q	1	2	Zero flow	Drainage rate Loss in drains Conc. at base
R,S,T	[a]Calculated	[c]Calculated	Zero flow	Drainage rate Loss in drains
U,V	[b]Calculated	[c]Calculated	Zero flow	Drainage rate Loss in drains
W	[a]Calculated	2	Percolation rate regulated by water table height	Percolation rate Leaching rate Drainage rate Loss in drains
X	[a]Calculated	2	Percolation rate regulated by water table height	Percolation rate Leaching rate Drainage rate Loss in drains
Y	[b]Calculated	2	Percolation rate regulated by water table height	Percolation rate Leaching rate Drainage rate Loss in drains

[a] minimum of: i.) depth to rock, ii.) profile depth
[b] minimum of: i.) depth to rock, ii.) depth to 'C' horizon, if texture= fine/medium iii.) 1 m
[c] minimum of: i.) depth to rock, or ii.) 2 m

Table 8 -Hydrologic classes as a basis for MACRO parameterisation.

The design water table height, *h*, is set to the drainage depth, or to 0.7 m, whichever is the smallest. In other words, for poorly drained sites, we assume that to achieve sustainability in agricultural systems (at least for those in which pesticides would typically be used), the drainage system (either natural or artificial) must be sufficient to prevent the water table from rising to the soil surface at the design discharge rate.

The design discharge is calculated as:

$$q_{eff} = P - q_{out} \tag{5}$$

where P is a design recharge rate (see below) and q_{out} is an average percolation rate at the base of the profile during the same period. The percolation rate q_{out} is obviously fixed at zero for the FOOTPRINT hydrological classes with zero flow as the bottom boundary condition, but it takes a positive value for the class with slowly permeable substrate (W, X and Y). Given the bottom boundary condition employed in MACRO for these hydrologic groups, to determine the drainage system design (i.e. spacing and depth of drains) q_{out} can be expressed as a linear function of the average water table height above the base of the soil profile H, under natural drainage conditions (i.e. in the absence of artificial drains):

$$q_{out} = B_{grad} H \tag{6}$$

where B_{grad} is the parameter (time constant) in the MACRO model (BGRAD) that controls percolation to groundwater. In FOOTPRINT, B_{grad} is estimated as:

$$B_{grad} = \frac{p_{gw} R}{H} \tag{7}$$

where R is the average percolation rate at the base of the profile (excess of precipitation over actual evapotranspiration) during the field capacity period and p_{gw} is the proportion of the excess water that percolates to groundwater. Thus, equation 5 can be re-written as:

$$q_{eff} = P - p_{gw} R \tag{8}$$

The parameter R obviously depends on climate and has been estimated for each of the FOOTPRINT climate zones by simple water balance modelling. The parameters p_{gw} and H are set in FOOTPRINT to reflect the original conceptual models underlying the HOST hydrologic classification system. For the sake of simplicity, p_{gw} and H are set to 0.5 and 0.5m respectively for hydrologic class W, and to 0.25 and 1.5m for classes X and Y. This implies that, in the same climate zone, B_{grad} is 6 times larger for class W than for X and Y. Table 9 shows the values of R and resulting values of B_{grad} (BGRAD) for each climate zone.

P should reflect a typical maximum amount of water recharging the water table on any day, and will therefore depend strongly on the depth of the water table in the soil (short-term peak flows in surface soil are 'damped out' with depth). Therefore, in FOOTPRINT, *P* is set to:

$$P = 20 \quad \text{for } z<0.5 \tag{9}$$

$$P = R \quad \text{for } z>(30-R)/20$$

$$\text{otherwise: } P = 30 - 20z$$

where *z* is the depth of the drainage base below the soil surface (in metres) and P and R are given in units of mm day^{-1}. This simple expression implies that *P* goes from a maximum of 20 mm day^{-1} for shallow lateral flow (i.e. drain depth of 0.5 m depth or less) to a minimum value equivalent to *R* if the drainage base is much deeper than 1 m.

FCZ	R (mm/day)	BGRAD	
		Class W	Class X and Y
1	1.93	8.0E-05	1.3E-05
2	1.47	6.1E-05	1.0E-05
3	2.38	9.9E-05	1.7E-05
4	1.14	4.8E-05	7.9E-06
6	6.55	2.7E-04	4.5E-05
7	2.58	1.1E-04	1.8E-05
8	2.64	1.1E-04	1.8E-05
9	2.98	1.2E-04	2.1E-05
10	1.25	5.2E-05	8.7E-06
11	2.94	1.2E-04	2.0E-05
12	5.93	2.5E-04	4.1E-05
13	5.93	2.5E-04	4.1E-05
14	1.23	5.1E-05	8.5E-06
15	0.99	4.1E-05	6.9E-06
16	1.91	8.0E-05	1.3E-05

Table 9 -Estimated values of R and BGRAD (1/hour) for slowly permeable substrates.

2.4 Crop parameters

Crop parameters (Tables 10, 11 and 12) are set for twelve different crop groups, partly according to FOCUS (2001) and partly based on information on drought tolerance and root depths in Allen et al. (1998). It should be noted that the maximum root depth shown in Tables 10 and 11 is reduced in the presence of a limiting soil horizon, following the decision rules in MACRO_DB (Jarvis et al., 1997). A horizon is considered limiting to root penetration if:

(‘C’ or ‘R’ horizon) or

(pH ≤ 4.5) or

((sand content (%)> 85- (silt content (%). 0.5)) and f_{oc} ≤ 0.2%) or

f_{st} > 0.2 or

(‘subsoil’ and ‘structure class = I’) and (bulk density > 1.65 g cm^{-3})

Parameter	Crop grouping								
	A	B	C	D	E	F	G	H	I
Maximum leaf area index (LAIMAX)	5	5	4	4	3	5	5	5	4
Green leaf area index at harvest (LAIHARV)	1	5	2	3	3	2	0.01	3	4
[a]Drought tolerance	Medium	Medium	Low	Medium	Low	Medium	Medium	High	Medium
Maximum root depth (m) (ROOTMAX)	1.1	0.8	0.5	0.8	0.5	1.1	1.4	1.1	0.8
Max. Interception capacity (mm) (CANCAP)	2	2	2	2	2	3	3	2	2
Ratio evaporation of intercepted water to transpiration (ZALP)	1.0	1.0	1.0	1.0	1.0	1.5	1.5	1.0	1.0

Table 10 -MACRO annual crop parameters.

A: Soft wheat, barley, rye, durum wheat, oats, flax, oilseed, rapeseed; B: Sugar beet, fodder root; C: Potato; D:Soya, pulses; E: Fresh vegetables; F: Maize grain, fodder maize, sunflower; G: Vineyards, orchards (deciduous); H: Cotton; I: Tobacco. [a] transpiration adaptability factor (BETA): low = 0.5, medium = 0.2, high = 0.1; critical tension for transpiration reduction (WATEN) is calculated from the known soil properties together with the % of extractable micropore water exhausted before reduction in transpiration occurs: low = 50%, medium = 65%, high = 80%

Parameter	Crop grouping		
	Grassland/ green fodder	Citrus	Olives
Leaf area index (LAIC)	5	5	3
[a]Drought tolerance	Medium	Medium	High
Root depth (m) (ROOTDEP)	0.8	1.4	1.4
Max. Interception capacity (mm) (CANCAP)	2	2	1
Ratio evaporation of intercepted water to transpiration (ZALP)	1.0	2.0	2.0

Table 11 -MACRO perennial crop parameters.

[a] transpiration adaptability factor (BETA): low=0.5, medium=0.2, high=0.1; critical tension for transpiration reduction (WATEN) calculated from known soil properties and the % of available water exhausted before reduction in transpiration occurs: low=50%, medium=65%, high=80%

For annual crops (groups A to I), specific dates of emergence, maximum leaf area and harvest are set for each crop grouping and FOOTPRINT climate zone.

Parameter	Value
Root distribution (RPIN)	67%
Leaf development factor, growth (CFORM)	1.6
Leaf development factor, senescence (DFORM)	0.3
Leaf area index on specified day[a] (LAIMIN)	0.01
Root depth on ZDATEMIN[a] (m) (ROOTINIT)	0.01
Critical air content for transpiration reduction (m^3 m^{-3}) (CRITAIR)	0.05

Table 12 -MACRO parameters constant for all crops.

[a] for spring-sown arable crops. For autumn-sown arable crops, LAIMIN and ROOTINIT are set to 1.0 and 0.2 respectively. For crop group G, ROOTINIT is set to 95% of the maximum root depth.

2.5 Solute transport

Apart from the diffusion pathlength (see section 2.1 of this chapter), all solute transport parameters are set to fixed values: the diffusion coefficient in water (DIFF) is set to the default value in FOCUS, namely 5×10^{-10} m^2 s^{-1}, the fraction of sorption sites in the macropores (FRACMAC) is set to 0.01, the mixing depth (ZMIX) is set to 1 mm and the anion exclusion water content (AEXC) to zero. In MACRO, the solute dispersivity (DV) is required to simulate dispersion in the soil matrix using the advection-dispersion equation. A few pedotransfer functions have been developed, but these have been based on experiments carried out on saturated soil (Gonçalves et al., 2001; Perfect et al., 2002) where macropores tend to dominate the observed dispersion. It would clearly not be appropriate to use such functions in conjunction with MACRO. Vanderborght and Vereecken (2007) recently described a database of dispersivities consisting of 635 values abstracted from 57 published studies. They showed that dispersivity tended to increase with the scale of the leaching experiment (from core to column to field), with flow rate, and with the distance travelled. An examination of a subset of the data presented by Vanderborght and Vereecken (2007) suggests that these effects are primarily due to preferential flow: we selected only those data (n = 116) obtained from experiments carried out at steady flow rates of less than 1 mm h^{-1}, since macropore flow could then reasonably be excluded (it should be noted that the subset analysed only contained experiments carried out on five texture classes with relatively small clay contents and, presumably, large K_{10} values i.e. sands, loamy sands, sandy loams, loams and silt loams). Even for this dataset, dispersivity was slightly (but not significantly) dependent on scale and transport distance. Omitting experiments carried out on small cores and for travel distances less than 50 cm, gave a median dispersivity of 3.4 cm, with no correlation to textural class. This value is used.

2.6 Validation

The use of pedotransfer routines introduces uncertainties into models predictions, which ideally should be quantified. Some of the functions used in FOOTPRINT are empirically well founded (e.g. the HYPRES functions) while others (i.e. the pedotransfer routines for macropore flow) are new and largely based on expert judgement. Two validation exercises were therefore carried out: i.) a test of the scheme to predict soil horizon susceptibility to macropore flow itself, independent of the MACRO parameterisation, and ii.) a test of the complete pedotransfer network to parameterise MACRO.

2.6.1 Model-independent validation

A version of the scheme shown in Figure 10, modified to account for tillage systems and traffic compaction (see Jarvis et al., 2009), was tested using data collated from the literature on tracer breakthrough in undisturbed soil columns (n=52). The breakthrough curves were scanned to estimate the pore volumes drained at the peak solute concentration, t_p, which was used as a measure of the strength of macropore flow. Analysis of variance for t_p as a function of susceptibility class showed that the overall model was significant (see Figure 12). It is concluded that macropore flow is predictable to a sufficient degree from easily available soil properties and site factors using the simple classification tree developed in FOOTPRINT.

2.6.2 Validation of the pedotransfer scheme for MACRO

The complete FOOTPRINT parameterisation scheme for MACRO was tested on a dataset of medium- to long-term outdoor lysimeter experiments consisting of 41 columns representing 15 soil types from 3 countries (Sweden, France, U.K.). Data on tracer leaching under natural climatic conditions was first compared to uncalibrated MACRO simulations. The results from some lysimeters were matched very well. However, not surprisingly, large errors were noted in other cases, related to both the timing and amount of water outflows and predicted rates of solute transport. A limited calibration exercise suggested that much of the error in the predictions was related to the estimation of evapotranspiration and root water uptake parameters and a failure to account for heterogeneous flow in the soil matrix in loamy soils. A 'benchmarking' validation exercise demonstrated that simulations were significantly poorer when macropore flow was excluded. Furthermore, Figure 13 shows that the relative ranking of the 15 soils for leaching at 0.1 pore volumes (i.e. early leaching that should be most relevant for pesticides) was reasonably well predicted by the 'blind' MACRO simulations, with a rank correlation coefficient which is significant at p=0.008. It is concluded that the FOOTPRINT methodology should provide a sound basis for predictions of the spatial distribution of pesticide leaching risks at the landscape scale.

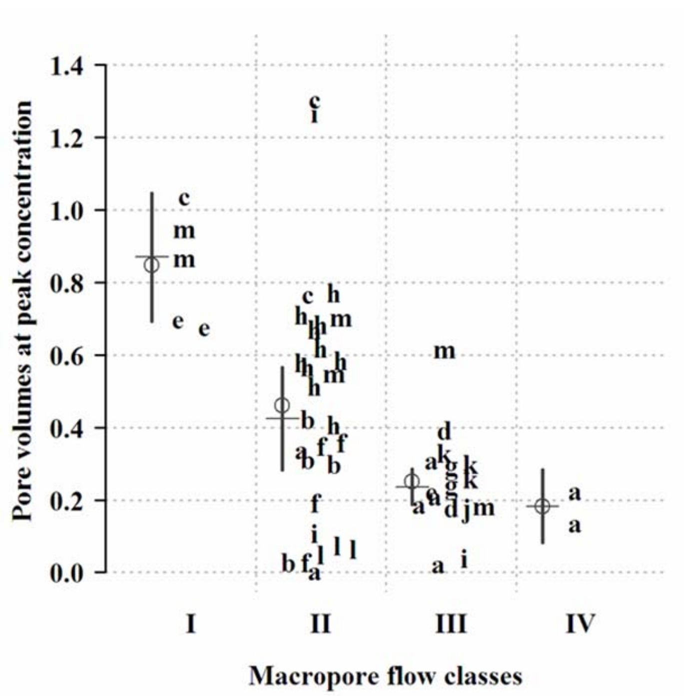


Figure 12 - tp as a function of predicted macropore flow class

Symbols are means, horizontal bars are medians. Vertical lines indicate confidence intervals for the median. Letters on the figure refer to individual studies.

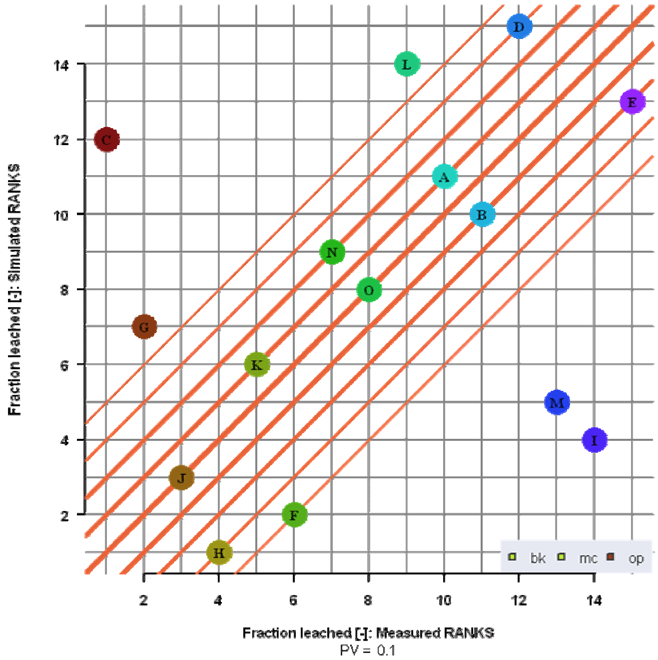


Figure 13 - Simulated and measured rankings for the fraction of solute leached at 0.1 pore volumes drained. Letters on the figure refer to individual soil types

3 PARAMETERISING THE PRZM MODEL

3.1 Summary

Section 3 of chapter 3 presents the results of work carried out within the FOOTPRINT project to develop a consistent and complete set of parameter estimation routines for the PRZM model (Carsel et al., 2003; FOCUS, 2001) that enable EU-wide simulations of pesticide losses from fields via surface runoff and erosion based on only readily available data (e.g. soil survey data and soil profile descriptions). The system is compatible with the data available at the EU level and the data farmers and extension advisors could gather quickly and at reasonable cost at the local field and farm scales.

PRZM is a 1-D pesticide fate model that is able to simulate pesticide losses from fields via surface runoff and erosion. PRZM is used in FOOTPRINT to make EU-wide predictions of pesticide inputs into surface waters via surface runoff and erosion.

Before employing PRZM in FOOTPRINT, a conceptual problem in PRZM had to be alleviated. PRZM uses the SCS Curve Number approach for the calculation of surface runoff. However, the SCS Curve Number Approach in fact calculates stream response to heavy rainfall events and thus implicitly includes all components of fast flow to surface water (so-called direct runoff; cf. Garen and Moore, 2005; NRCS, 2004): infiltration excess runoff, saturation excess runoff, lateral subsurface flow, channel runoff (this is rainfall directly falling on water bodies; can be neglected here) and, where applicable, drainflow. In PRZM, the SCS Curve Number approach is implemented in a conceptually wrong way: all direct runoff calculated with the CN approach is treated as infiltration excess runoff. For this reason, we adjusted the USDA soil hydrologic groups (which determine the curve numbers and thus the frequency and magnitude of runoff events) this way that they only reflect surface runoff (infiltration excess runoff + saturation excess runoff). Lateral subsurface flow is calculated with the model MACRO.

Several data sources are used to support the calculation of model parameters: the Soil Geographic Database of Europe, v. 1.0 (Le Bas et al., 1998) was used to identify 264 'benchmark' soil profiles ('FOOTPRINT soil types') that characterise agricultural land in Europe. The following data, which were derived from the SPADE-1 and -2 databases (see Chapter 2, section 2.6) for each soil horizon, were used to support the parameterization of hydraulic properties in the model: horizon designation; upper depth (cm); lower depth (cm); clay, silt and sand (%); stone content (%); pH (H_2O); organic carbon content (%); bulk density (kg dm^{-3}). Each soil type is classified into one of 15 unique hydrological classes based on the HOST ('Hydrology of Soil Types') system, the FOOTPRINT hydrologic groups (FHG). These determine the USDA hydrologic group and thus the curve numbers.

For parameters other than basic soil property data and soil hydrologic group, the runoff and erosion model PRZM was parameterised using both the parameterisation guidance in the PRZM 3.12.1 manual (Carsel et al., 2003) and in the FOCUS surface water report (FOCUS, 2001). Crop parameters were harmonized with the crop parameters used in MACRO within FOOTPRINT.

3.2 Process descriptions in PRZM

PRZM (**P**esticide **R**oot **Z**one **M**odel) 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 (Carsel et al., 2003). The original version of the PRZM model was released in 1984 (Carsel et al., 1984). The model has been continuously improved since then. The latest, Windows-based version PRZM 3.21β is used in the context of the FOCUS surface water scenarios (FOCUS, 2001) as runoff and erosion model. A version with only minor differences is also used as one of the official leaching models in the FOCUS groundwater scenarios (FOCUS, 2000).

The PRZM model is able to simulate surface runoff, erosion, leaching, decay, plant uptake, foliar washoff, and volatilisation of pesticides. It has two major components – water and chemical transport. In the following, the processes of PRZM relevant for runoff and erosion modelling are explained briefly.

3.2.1 Water Transport

PRZM is a capacity-type model with a daily time step. Water movement is simulated with a rather simple approach. The soil profile is divided into several layers. A soil layer is characterized by three hydraulic parameters: field capacity (usually reported as the amount of water the soil can hold against the influence of gravity), wilting point (the soil moisture content below which plants can no longer extract water from the soil), and saturated water content (pore volume). If the soil water content of a soil layer exceeds field capacity, the excess water drains to the next layer. The whole soil profile drains within one day to field capacity. Thus, PRZM is not able to simulate waterlogging. As PRZM is also unable to simulate preferential flow, its application should be restricted to well-drained soils without strongly developed soil structure if leaching estimates are required. However, since waterlogging rarely occurs in the topsoil and leaching by preferential flow does not significantly affect bulk pesticide concentrations in the topsoil, these limitations do not affect the general applicability of PRZM to runoff and erosion problems.

Evapotranspiration in PRZM is composed of evaporation from crop interception, evaporation from soil and transpiration from the crop. Potential evapotranspiration is obtained from direct input of daily pan evaporation, multiplied with a crop-specific correction factor.

PRZM is not able to simulate upward water movement due to hydraulic potential gradients induced by evapotranspiration. This can lead to an underestimation of actual evapo-transpiration.

Surface runoff is described by a modification of the empirical USDA Soil Conservation Service (SCS) Curve Number technique (Haith and Loehr, 1979):

$$Q = \frac{(P + SM - 0.2S)^2}{P + SM + 0.8S} \qquad \text{for } (P + SM - 0.2\,S) > 0 \qquad (10)$$

$$Q = 0 \qquad \text{for } (P + SM - 0.2\,S) \leq 0$$

where

Q surface runoff (cm d^{-1})

P precipitation as rainfall, minus crop interception (cm d^{-1})

SM snowmelt (cm d^{-1})

S daily watershed retention parameter (cm d^{-1}); 0.2 S is also referred to as “initial abstraction”

The daily watershed retention parameter S (cm d^{-1}) is estimated by

$$S = 2.54 * \left(\frac{1000}{CN} - 10 \right) \quad (11)$$

with

CN	SCS runoff curve number ($0 < CN \leq 100$)
2.54	unit conversion factor that converts inches to cm

Curve numbers are a function of soil type, soil drainage properties, crop type and management practice (Carsel et al., 2003). The higher the curve number, the more frequently runoff will occur, and the higher the runoff volume per event will be. In PRZM, the curve numbers are adjusted daily as a function of the soil water status in the upper soil layers, following the algorithms developed and reported by Haith and Loehr (1979). Runoff curve numbers are tabulated for different crops and soil hydrologic groups in the PRZM 3.12.1 Manual (Carsel et al., 2003). Curve numbers and thus runoff susceptibility increase from group A (light, sandy soils) to D (heavy, clayey soils). Note that although PRZM considers the effect of snowmelt in the runoff equation, the curve numbers are not adjusted to account for the effects of snowpack or frozen ground on runoff generation.

Soil loss by sheet and rill erosion is also modelled empirically in PRZM using the Modified Universal Soil Loss Equation (MUSLE; Williams, 1975) or one of its modifications (MUSS, MUST). MUSS was specifically designed for small watersheds and is used in the PRZM calculations in the FOCUS surface water scenarios.

$$\text{MUSLE: } X_e = 1.586\ (V_r\ q_p)^{0.56}\ A^{0.12}\ K\ LS\ C\ P \quad (12)$$

$$\text{MUSS: } X_e = 0.79\ (V_r\ q_p)^{0.65}\ A^{0.009}\ K\ LS\ C\ P \quad (13)$$

where

X_e	event soil loss (t d^{-1})
V_r	volume of event (daily) runoff (mm)
q_p	peak storm runoff rate (mm h^{-1})
A	field size (ha)
K	soil erodibility factor (dimensionless)
LS	length-slope factor (dimensionless)
C	soil cover factor = crop management factor (dimensionless)
P	conservation practice factor (dimensionless)

While *A*, *K*, *LS*, *C* and *P* are user input, q_p is calculated internally in PRZM, using a generic storm hydrograph. The rainfall intensity is assumed to occur according to “design storm distributions” or rainfall regimes. The rainfall regime is entered by the PRZM user. For Western and Middle Europe, type II, which covers the largest part of the USA without the Atlantic, Pacific and southern regions, is the most appropriate rainfall regime.

3.2.2 Pesticide Transport and Fate

In contrast to the older PRZM version 3.12 used by the US Environmental Protection Agency (Carsel et al., 2003), the version 3.21β (which was developed specifically for the use in FOCUS surface water) is also capable of modelling non-linear sorption and temperature- and moisture-dependent degradation (FOCUS, 2001). Sorption is described identically as in MACRO using a Freundlich isotherm. Degradation is by default described by single first-order kinetics; however, there is also a possibility to specify biphasic degradation with a “hockey-stick” model, which switches from a fast first-order kinetic to a slower one at a user-defined time point.

The temperature dependence of degradation is based on a Q_{10} equation, which is mathematically equivalent to the formula used in MACRO as an approximation of the Arrhenius equation. The moisture-dependence of degradation is also in PRZM described with the Walker formula. However, in PRZM the reference moisture can be freely chosen, either as absolute volumetric moisture or in percent of field capacity.

The extraction of pesticides from soil with runoff water follows an empirical approach, where the runoff-availability of a compound decreases with depth (“non-uniform extraction model”; Carsel et al., 2003):

$$DRI_i = 0.7 \cdot \left(\frac{1}{2.0 \cdot Midtot_i + 0.9} \right)^2 \tag{14}$$

where

DRI$_i$ fraction of dissolved-phase chemical present in compartment i available for runoff (dimensionless)

Midtot$_i$ depth to midpoint of compartment i (cm)

0.7 efficiency factor

0.9 depth-reduction coefficient

Calculations are performed for all compartments *i* from the surface to a depth of 2 cm; the thickness of the topsoil compartments is usually set to 0.1 cm. Thus, the runoff-available fraction decreases from 70 % of the dissolved chemical in the uppermost compartment to 3 % in the 20^{th} compartment. Below 2 cm depth the runoff availability of chemicals is zero. Pesticide runoff loss from compartment *i* is then obtained as

$$J_{r,i} = DRI_i \cdot C_i \cdot Q \cdot 10 \quad (15)$$

with

$J_{r,i}$ pesticide runoff loss from compartment i (mg m^{-2} d^{-1})

C_i concentration of dissolved pesticide in the water phase (mg L^{-1})

10 unit correction factor

During erosion events, apart from losses dissolved in surface runoff, pesticides can also leave the field adsorbed to eroded topsoil material. Because erosion is a selective process, eroded soil material is, compared with the topsoil from which it was eroded, enriched in smaller particles and organic matter (the main sorbent for non-ionic pesticides). In PRZM, the enrichment ratio for organic matter r_{om} is calculated empirically according to the following equation:

$$\ln (r_{om}) = 2 - 0.2 \ln (1000\, X_e/A) \quad (16)$$

Thus, larger erosion events are less selective and will result in lesser enrichment of organic matter. Pesticide loss from the field via erosion is calculated as

$$J_e = \frac{X_e \cdot r_{om} \cdot S_1}{10 \cdot A} \quad (17)$$

with

J_e pesticide erosion loss (mg m^{-2} d^{-1})

S_1 concentration of adsorbed pesticide in the solid phase (mg kg^{-1}) in the uppermost compartment

10 unit correction factor

In contrast to MACRO, PRZM is also able to model pesticide losses via volatilization. PRZM explicitly simulates vapour phase diffusion in soil, volatilization from soil and plant surfaces, and volatilization flux through the plant canopy. A detailed process description cannot be given here, but can be found in Carsel et al. (2003). Pesticide washoff from the crop canopy to the soil surface is modelled using an empirical extraction coefficient Pesticide uptake by roots is treated in the same way as in MACRO as a passive process with a plant uptake concentration factor between 0 and 1.

3.3 Parameterisation of PRZM

The PRZM model is in principle straightforward to parameterise. However, the input file (.inp) contains a lot of switches and flags whose values have to be set carefully if meaningful results are to be produced. For this reason, the rules used in FOOTPRINT to parameterise the PRZM model are given in tabular form for each record and input parameter of the .inp file (Table 13). Further details are given in an xls file produced as part of DL20 (Reichenberger et al., 2008a). This file contains the full set of PRZM input parameters for 15 FOOTPRINT climate zones (FCZ), 264 agriculturally relevant FOOTPRINT soil types (FST) and 42 FOOTPRINT crops (FCR).

Record	Parameter name	Description	FOOTRINT parameterisation
1	TITLE	Label for simulation title	Set to the FOOTPRINT Unique Numbering. Uniquely identifies each of the FOOTPRINT model runs
2	HTITLE	Label for hydrology information title	N/A
3	PFAC	Pan factor used to estimate daily evapotranspiration	Set to 1 since PET is fed directly.
3	SFAC	Snowmelt factor in cm/°C	Set to 0.46 (default value from FOCUSgw)
3	IPEIND	Pan factor flag	Set to 0 (pan data read)
3	ANETD	Minimum depth of which evapotranspiration is extracted (cm); the value of ANETD applies when the soil is bare and only evaporation can occur	Depending on climate zone; Rules used: (arbitrary, following FOCUS) annual Tmean ANETD < 5 °C 10 5 - < 9.5 °C 15 9.5 - > 13 °C 20 13 - < 16 °C 25 >= 16 °C 30 Results: FCZ ANETD 1 20 2 20 3 15 4 10 5 20 6 15 7 20 8 30 9 30 10 10 11 25 12 15

			14 15 15 15 16 15
3	INICRP	Indicates the initial crop if the simulation start date occurs before the emergence date of the first crop	1 (in theory, only used if erosion is switched off; however, if INICRP is set to zero, PRZM operates wrongly)
3	ISCOND	Surface condition of initial crop	1 (in theory, only used if erosion is switched off; set according to FOCUSsw)
6	ERFLAG	Flag to calculate erosion	Set to 4 in accordance with FOCUSsw (MUSS approach)
7	USLEK	soil erodibility factor K of the Universal Soil Loss Equation (USLE) and its modifications (MUSLE/MUSS)	Calculated for each of the 264 FSTs. The PRZM 3.12.1 Manual (Carsel et al., 2003) lists values of USLEK for different combinations of USDA texture class and 3 levels of OM content (< 0.5, 2 and 4 %). Unfortunately, the manual doesn't give class boundaries; hence we set the class boundaries to 1 % and 3 % OM, yielding three classes: 0 - < 1 % OM, 1 - < 3 % OM, >= 3 % OM. For each FST, the USDA texture class and the OM class of the uppermost horizon were determined. Subsequently, the USLEK value for the respective texture class / OM class combination was assigned to each FST. USLEK values for FSTs with organic topsoils were set to 0.01 (topsoil with 50 % OC) and 0.02 (topsoil with 26 % OC).
7	USLELS	Topographic factor LS of the USLE (combined slope length / steepness factor)	Calculated according to the SWAT2005 Theory (Neitsch et al., 2005) with the following formula: $USLELS = (L_{hill}/22.1)^{m} * (65.41 * \sin^{2}(\alpha_{hill}) + 4.56 \sin(\alpha_{hill}) + 0.065)$ Where L_{hill} is the slope length (m); set to 100 m in FOOTPRINT α_{hill} is the angle of the slope (rad); set specifically for each FST The exponent m is calculated as follows: $m = 0.6 (1 – \exp(-25.835 * slp))$ where slp is the slope expressed as a fraction ($slp = \tan \alpha_{hill}$)
7	USLEP	Erosion control	Calculated FST-specifically according to the PRZM 3.12.1 Manual (Carsel et al., 2003). Contouring is assumed.

<table>
<tr><td></td><td></td><td>practice factor of the USLE</td><td><table><tr><th>FST slope (%)</th><th>USLEP</th></tr><tr><td>0 - 2</td><td>0.6</td></tr><tr><td>> 2 - 7</td><td>0.5</td></tr><tr><td>> 7 – 12</td><td>0.6</td></tr><tr><td>> 12</td><td>0.8</td></tr></table></td></tr>
<tr><td>7</td><td>AFIELD</td><td>Field area (ha)</td><td>Set to 1</td></tr>
<tr><td>7</td><td>IREG</td><td>Type of rainfall intensity distribution</td><td>Different values specified for each of the 16 FCZ. PRZM does not allow to specify intensity distributions directly. One can only choose between different rainfall intensity regimes.
The different IREG in PRZM denote the following:
<table>
<tr><th></th><th></th><th colspan="2">distributions assigned</th></tr>
<tr><th>IREG</th><th>occurrence in US</th><th>summer (01/05 - 15/09)</th><th>winter (16/09 - 30/04)</th></tr>
<tr><td>1</td><td>Southern California, Alaska, Hawaii</td><td>Type I</td><td>Type I A</td></tr>
<tr><td>2</td><td>NW coast</td><td>Type I A</td><td>Type I A</td></tr>
<tr><td>3</td><td>rest of US</td><td>Type II</td><td>Type I A; for events > 5.08 cm/d Type I is used</td></tr>
<tr><td>4</td><td>Gulf region, Florida, east coast</td><td>Type III</td><td>Type I A; for events > 5.08 cm/d Type I is used</td></tr>
</table>
<table>
<tr><th>IREG</th><th>Interpretation</th><th>suitable for which European regions</th></tr>
<tr><td>1</td><td>intermediate intensity in summer, low intensity in winter</td><td>Transitional climates</td></tr>
<tr><td>2</td><td>Always low intensity</td><td>Northern + Western Europe</td></tr>
<tr><td>3</td><td>high intensity in summer, low and (for larger events) intermediate in winter</td><td>Central Europe + Mediterranean</td></tr>
<tr><td>4</td><td>rather high intensity in summer, low and (for larger events) intermediate in winter</td><td>no such climate (subtropical east-coast) in Europe</td></tr>
</table>
As a result, IREG was assigned to each FCZ as follows:
<table>
<tr><th>FCZ</th><th>IREG</th></tr>
<tr><td>1</td><td>3</td></tr>
<tr><td>2</td><td>1</td></tr>
<tr><td>3</td><td>3</td></tr>
<tr><td>4</td><td>2</td></tr>
</table></td></tr>
</table>

			5 1 6 3 7 2 8 3 9 3 10 2 11 2 12 2 14 3 15 1 16 2
7	SLP	Land slope (%)	Different values specified for each of the 264 FSTs. First, descriptive statistics (mean, median, min, max etc.) on slopes from a European slope map (provided by O. Cerdan, BRGM) were calculated for each Soil Map Unit (SMU) in the SGDBE. These statistics were used by John Hollis to derive a 'best estimate' average slope for each FST with an arable or permanent crop land use (as indicated by the USE1 & USE2 attributes in the STU.dbf file of the SGDBE).In most cases the estimated slopes were based on the calculated median slope and 'majority' slope of the SMU in which the FST occurs. However, the estimated slopes were adjusted using a 'weighting' parameter based on the fraction of cover of the STU within the SMU multiplied by the calculated area of each SMU used to derive the slope statistics. In a significant number of cases though, the FST did not represent a significant enough fraction of the SMU area used to calculate the slope data for the slope statistics to be relevant. In such cases the slope was estimated either using expert judgement based on the range of soils within the SMU and the calculated slope statistics, or by using the data on slope ranges (SLOPE1 & SLOPE2) given in STU.dbf file of the SGDBE.
7	HL	Hydraulic length (m)	Denotes the length from the most distant point of the field to the field outlet. Assuming a square field of 1 ha area with the outlet in the middle of the lower field boundary yields a hydraulic length of 111.8 m.
8	NDC	Number of different crops in the simulation	Set to 1 (no crop rotation).
9	ICNCN	Crop number of the different crop	Set to 1 (there is only one crop)
9	CINTCP	Maximum interception storage of the crop (cm)	Set specifically for each FOOTPRINT crop (FCR) in accordance with the MACRO parameterization. The corresponding MACRO parameter is CANCAP (mm).

9	AMXDR	Maximum rooting depth of the crop (cm)	Set specifically for each combination of FOOTPRINT crop (FCR) and FOOTPRINT soil type (FST) in accordance with the MACRO parameterization. The corresponding MACRO parameters are ROOTMAX (annual crops, m) and ROOTDEP (perennial crops, m). AMXDR is computed as the minimum of the crop-inherent maximum rooting depth and the depth to the uppermost root-limiting horizon in the soil profile. The rules for determining whether a horizon is root-limiting or not are: 1. the topsoil horizon (number 1) can never be limiting to root growth, regardless of its properties 2. a subsoil horizon must be at least 25 cm thick if it is to restrict root growth 3. one or more of the following criteria must be fulfilled: - horizon designation C or R - pH (H_2O) <= 4.5 - sand% > (85 - silt% * 0.5) AND OC content <= 0.2 % - volumetric stone content > 20 % - structure class * = I AND bulk density > 1.65 g cm^{-3} * for structure classes cf. DL21)
9	COVMAX	Maximum areic coverage of the canopy (%)	Source of COVMAX for bush berries, flax, strawberries, tomatoes: FOCUSgw (FOCUS, 2000). These are the crops not occurring in FOCUS surface water. Source of COVMAX for all other crops: FOCUSsw (FOCUS, 2001)
9	ICNAH	Surface condition of the crop after harvest date	Set to 3 (= residue) in accordance with FOCUSsw. This parameter is allegedly only used when erosion is switched off.
9	CN1		Set to 0 (only used if erosion is switched off → not used here)
9	CN2		Set to 0 (only used if erosion is switched off → not used here)
9	CN3		Set to 0 (only used if erosion is switched off → not used here)
9	WFMAX		Set to 0 (only used if CAM = 3 → not used here)
9	HTMAX	Max. canopy height at maturation date (cm)	Set specifically for each FOOTPRINT crop. Derived from FOCUSsw PRZM and MACRO parameterization of crop height (they considerably differ from each other!) and expert judgement.
9A	CROPNO	Crop number	Set to 1 (there is only one crop)
9A	NUSLEC	Number of USLEC	Set to 6 (the 4 cropping dates in FOCUSsw turned out too few, because in FOCUSsw the curve number decreases sharply at emergence date from the value for fallow to the value for a fully developed crop).

<table>
<tr><td></td><td></td><td>factors (and CN and cropping dates)</td><td></td></tr>
<tr><td>9B</td><td>GDUSLEC</td><td>Day to start USLEC, MNGN and CN. The first date has to be the crop emergence date.</td><td>Set specifically for each combination of FCR and FCZ. Since NUSLEC = 6, 6 values for GDUSLEC are required. The 6 crop dates denote the following:
GDUSLEC/GMUSLEC 1 corresponds to emergence
GDUSLEC/GMUSLEC 2 corresponds to ZDATEMIN in MACRO (the point where the crop development becomes faster, matters for winter crops)
GDUSLEC/GMUSLEC 3 corresponds to intermediate development (e.g. half of maximum ground cover)
GDUSLEC/GMUSLEC 4 corresponds to maturity
GDUSLEC/GMUSLEC 5 corresponds to harvest
GDUSLEC/GMUSLEC 6 corresponds to removal of residues
Values were obtained using NUTS2-specific cropping dates collected by all FOOTPRINT partners.</td></tr>
<tr><td>9B</td><td>GMUSLEC</td><td>Month to start USLEC, MNGN and CN. The first date has to be the crop emergence date.</td><td>Set specifically for each combination of FCR and FCZ. Since NUSLEC = 6, 6 values for GDUSLEC are required. The 6 crop dates denote the following:
GDUSLEC/GMUSLEC 1 corresponds to emergence
GDUSLEC/GMUSLEC 2 corresponds to ZDATEMIN in MACRO (the point where the crop development becomes faster, matters for winter crops)
GDUSLEC/GMUSLEC 3 corresponds to intermediate development (e.g. half of maximum ground cover)
GDUSLEC/GMUSLEC 4 corresponds to maturity
GDUSLEC/GMUSLEC 5 corresponds to harvest
GDUSLEC/GMUSLEC 6 corresponds to removal of residues
Values were obtained using NUTS2-specific cropping dates collected by all FOOTPRINT partners.</td></tr>
<tr><td>9C</td><td>USLEC</td><td>Cover management factors C of the USLE for the different crop stages</td><td>Set specifically for each FOOTPRINT crop. Since NUSLEC = 6, 6 values for USLEC are required. The USLEC were set as follows:
<table>
<tr><th>crop type</th><th>USLEC1</th><th>USLEC2</th><th>USLEC3</th><th>USLEC4</th><th>USLEC5</th><th>USLEC6</th></tr>
<tr><td>grass/greenfodder</td><td>0.02</td><td>0.02</td><td>0.02</td><td>0.02</td><td>0.02</td><td>0.02</td></tr>
<tr><td>other permanent crops</td><td>0.2</td><td>0.2</td><td>0.2</td><td>0.2</td><td>0.2</td><td>0.2</td></tr>
<tr><td>annual crops</td><td>0.6</td><td>0.4</td><td>0.3</td><td>0.2</td><td>0.4</td><td>0.9</td></tr>
</table></td></tr>
<tr><td>9D</td><td>MNGN</td><td>Manning's roughness coefficient for the different crop stages (apparently unitless)</td><td>Set constant to 0.10, in accordance with FOCUSsw.</td></tr>
</table>

9E	CN	SCS runoff curve numbers (for antecedent moisture condition II) for the different crop stages	In PRZM, the SCS Curve Number approach is implemented in a conceptually wrong way (cf. Garen and Moore, 2005): all direct runoff calculated with the CN approach is treated as infiltration excess runoff. For this reason, we adjusted the USDA soil hydrologic groups (which determine the curve numbers and thus the frequency and magnitude of runoff events) for each FOOTPRINT hydrologic group (FHG) this way that they only reflect surface runoff (infiltration excess runoff + saturation excess runoff). Possible lateral subsurface flow occurring in a given FHG is calculated with the model MACRO. The CN were set specifically for each combination of PRZM soil hydrologic group, FCR and crop stage. The set of Curve Numbers was obtained in 3 steps: 1. The PRZM soil hydrologic group (A, B, B-C, C, D) is determined by the FOOTPRINT hydrologic group. Hence, each FST has a PRZM soil hydrologic group attached to it. PRZM soil hydrologic groups have been adjusted this way that PRZM only calculates surface runoff (while the CN approach originally calculates total direct runoff). 2. The PRZM 3.12.1 Manual lists curve numbers for different PRZM soil hydrologic groups and different combinations of crop group (the CN are for a fully developed crop), agricultural practice and hydrologic condition (e.g. “small grain, contoured, good” and. Each FCR was assigned one of these combinations. → set of curve numbers for each combination of FST and FCR, for fully developed crop and fallow condition. 3. Linear interpolation of CN for the other crop stages according to the following equations: CN1 = CN_fallow - 0.25 (CN_fallow - CN_crop) = 0.75 CN_fallow + 0.25 CN_crop CN2 = CN_fallow - 0.5 (CN_fallow - CN_crop) = 0.5 CN_fallow + 0.5 CN_crop CN3 = CN_fallow - 0.75 (CN_fallow - CN_crop) = 0.25 CN_fallow + 0.75 CN_crop CN4 = CN_crop CN5 = CN_fallow - 0.5 (CN_fallow - CN_crop) = 0.5 CN_fallow + 0.5 CN_crop CN6 = CN_fallow
10	NCPDS	Number of cropping periods	Set to 26 (includes 6 warmup years for eventual buildup of residues)
11	EMD	Integer day of crop emergence	Set to same value as GDUSLEC1 for each cropping period
11	EMM	Integer month of crop emergence	Set to same value as GMUSLEC1 for each cropping period
11	IYREM	Integer year of crop emergence	Enter last two digits of each simulation year. The simulation period has to be adjusted such that there are no problems with the year 2000 (PRZM cannot handle it because the year has only two digits) or with leap years.

11	MAD	Integer day of crop maturation	Set to same value as GDUSLEC4 for each cropping period
11	MAM	Integer month of crop maturation	Set to same value as GMUSLEC4 for each cropping period
11	IYRMAT	Integer year of crop maturation	Enter last two digits of each simulation year. The simulation period has to be adjusted such that there are no problems with the year 2000 (PRZM cannot handle it because the year has only two digits) or with leap years.
11	HAD	Integer day of crop harvest	Set to same value as GDUSLEC5 for each cropping period
11	HAM	Integer month of crop harvest	Set to same value as GMUSLEC5 for each cropping period
11	IYRHAR	Integer year of crop harvest	Enter last two digits of each simulation year. The simulation period has to be adjusted such that there are no problems with the year 2000 (PRZM cannot handle it because the year has only two digits) or with leap years.
11	INCROP	Crop number	Set to 1 (there is only one crop)
12	PTITLE	Label for pesticide title	String composed of Koc reference, DT50 reference, crop reference and application month reference
13	NAPS	Total number of pesticide applications occurring at different dates	Set to 26 (one application per year).
13	NCHEM	Number of pesticides in the simulation	Set to 1.
13	FRMFLG	Flag for testing of ideal soil moisture conditions for the application of pesticides relative to	Set to 0 (no testing) in accordance with FOCUSsw.

		the target date	
13	DKFLG2	Flag to allow input of biphasic degradation behaviour	Set to 0 (corresponds to FOCUS default).
15	PSTNAM	Name of pesticide for output titles	String composed of Koc reference, Koc value (in parentheses), DT50 reference and DT50 value (in parentheses)
16	APD	Integer target application day	Application date is determined based on the rainfall pattern in the application month with the following procedure: 1. Start with day 15 of the month 2. IF (Less than 20mm of rainfall the preceding day) AND (Less than 5mm of rainfall the 9 hours preceding application) THEN Application day 3. If conditions not satisifed, try day 14, then 16, then 13, then 17 and so on
16	AMD	Integer target application month	Set to the same value for each application year.
16	IAPYR	Integer target application year	Pesticides are applied once per simulation year.
16	WINDAY	Number of days in which to check soil moisture values following the target date for ideal pesticide applications	Set to zero (not used)
16	CAM	Chemical application method	Set to 2 (interception based on crop canopy, as a straight-line function of crop development; chemical reaching the soil is incorporated to 4 cm depth with concentration linearly decreasing with depth.
16	DEPI	Depth of the pesticide application (cm)	Set to 0 (not used if CAM = 2)

16	TAPP	Target application rate of the pesticide (kg ha^{-1})	Set to 1.
16	APPEFF	Application efficiency (fraction)	Set to 1 (in accordance with FOCUS).
16	DRFT	Spray drift (fraction).	Set to 0 (in accordance with FOCUSsw). In FOOTPRINT, drift is calculated outside PRZM.
17	FILTRA	Filtration parameter	Set to 0 (not used if CAM = 2)
17	IPSCND	Condition of foliar pesticide after harvest.	Set to 2 (2 = complete removal). Makes more sense than FOCUS setting (1 = surface applied).
17	UPTKF	Plant uptake factor	Set to 0.5 (FOCUSsw default for systemic pesticides). Yet, also non-systemic pesticides may be taken up by roots with the transpiration flux (they are just not translocated within the plant). The default value of 0.5 can therefore be used for all nonionic pesticides.
18	PLVKRT	Pesticide volatilization rate constant on plant foliage (d^{-1})	Set to 0 (in accordance with FOCUSsw).
18	PLDKRT	Pesticide decay rate constant on plant foliage (d^{-1})	Set to 0.06932 (corresponding to a foliar half-life of 10 days). This parameter is used in FOOTPRINT and FOCUS as a lumped dissipation rate constant (including also volatilization).
19	FEXTRC	Foliar extraction coefficient (cm^{-1}) for pesticide washoff per centimeter of rainfall	Set to 0.5 (FOCUSsw recommendation in absence of data on water solubility).
19	STITLE	Label for soil properties title	Set to the FOOTPRINT Unique Numbering. Uniquely identifies each of the FOOTPRINT model runs
20	CORED	Total depth of soil	Set FST-specifically. Hard rock horizons are excluded from CORED.

		core (cm)	
20	BDFLAG	Bulk density flag	Set to 0 in accordance with FOCUSsw (bulk density directly entered in record 33).
20	THFLAG	Field capacity and wilting point flag	Set to 0 in accordance with FOCUSsw (water contents are directly entered in record 37).
20	KDFLAG	Soil adsorption flag	Set to 2 in accordance with FOCUSsw (normalized Freundlich equation).
20	HSWZT	Drainage flag	Set to 0 in accordance with FOCUSsw (free drainage). Restricted drainage would be interesting for some soils but this piece of code doesn't work.
20	MOC	Method of char-acteristics flag	Set to 0 in accordance with FOCUSsw (MOC not used).
20	IRFLAG	Irrigation flag	Set to 0 in accordance with FOCUSsw (irrigation not simulated). In FOOTPRINT and FOCUS, irrigation is included in the rainfall time series.
20	ITFLAG	Soil temperature simulation flag	Set to 2 (temperature- and moisture-dependent degradation rate). This option is used in FOCUSsw when laboratory degradation data are used.
20	IDFLAG	Thermal conductivity and heat capacity flag	Set to 1 in accordance with FOCUSsw (PRZM simulates temperature profile using default thermal conductivity and heat capacity, calculated from basic soil horizon properties, e.g. texture and organic carbon content).
20	BIOFLG	Biodegradation flag	Set to 0 in accordance with FOCUSsw (microbial population degradation algorithms not used).
26	DAIR	Diffusion coefficient for the pesticide in air (cm^2 d^{-1})	Set to 4300 in accordance with FOCUSsw.
26	HENRYK	Henry's Law constant of the pesticide (dimensionless)	Set to 0 (leads to zero volatilization). Since we simulate dummy substances, we can only make assumptions on Henry's Law constant. The assumption of no volatilization is a conservative one and therefore more appropriate in this case than the choice of a hypothetical HENRYK value > 0.
26	ENPY	Enthalpy of vaporization of the pesticide (kcal mol^{-1})	Set to 22.7 in accordance with FOCUSsw.

30A	FRNDCF	Freundlich exponent	Set to 1 (linear sorption). For the metamodelling, nonlinear sorption could not be considered, because then sorption would also depend on the application rate. → Additional to Koc and DT50, two more dimensions (Freundlich exponent and application rate) would have been necessary to create the metamodel database.
31	ALBEDO	Monthly values of soil surface albedo	Set to 0.18 for each month in accordance with FOCUSsw.
31	EMMISS	Emissivity of the soil surface for longwave radiation (fraction)	Set to 0.96 in accordance with FOCUS:
31	ZWIND	Height of wind speed measurement above the soil surface (m)	Set to 10 m, which corresponds to the weather stations whose data were used to generate the PRZM met files.
32	BBT	Average monthly values of soil temperatures (°C) at the bottom boundary of the profile	Set to annual average air temperature in accordance with FOCUS.
32A	QFAC	Q_{10} factor for degradation rate increase when temperature in-creases by 10 °C	Set to 2.2 in accordance with FOCUSsw (corresponding to an activation energy of 54 KJ mol^{-1})
32A	TBASE	Reference temperature for entered degradation rate constants	Set to 20 °C (most common value in degradation studies).

32B	ABSREL	Flag for type of reference soil moisture (absolute or relative to FC)	Set to 2 (= relative; i.e. values are entered in % of field capacity)
32B	B-VALUE	Exponent for moisture correction of degradation rate	Set to 0.7 (FOCUSsw default value).
32B	REFMOIST	Reference soil moisture for moisture correction of degradation rate	Set to 100 (= 100 % of field capacity)
33	NHORIZ	Total number of horizons	Specific for each FST. Horizons with upper boundary > 10 cm depth and lower boundary < 10 cm depth were split in two at 10 cm depth.
Note: Records 34-38 are to be entered in blocks for each horizon. First, the uppermost horizon is specified completely, then the next one, and so on.			
34	HORIZN	Horizon number	(running from 1 to NHORIZ)
34	THKNS	Thickness of the horizon	FST- and horizon-specific. Note that horizon boundary depths (and thus thickness) beyond 10 cm soil depth have been rounded to multiples of 5 cm. This was necessary because the numerical layers below 10 cm soil depth are 5 cm thick.
34	BD	Dry bulk density (g cm^{-3})	FST- and horizon-specific.
34	THETO	Initial volumetric soil water content in the horizon (cm^3 cm^{-3})	Set equal to field capacity (parameter THEFC) in accordance with FOCUSsw.
34	AD	Soil drainage parameter (d^{-1})	Set to 0 in accordance with FOCUSsw (option not used).
34	DISP	Pesticide hydro-dynamic dispers-ion coefficient (cm^2 d^{-1})	Set to 0 in accordance with FOCUSsw (dispersion is simulated numerically).
34	ADL	Lateral soil drainage	Set to 0 in accordance with FOCUSsw (option not used).

		parameter (d^{-1})	
36	DWRATE	Dissolved phase pesticide degradation rate constant (d^{-1})	Specific for each dummy substance (ln2 / DT50). Correction of degradation rates with depth is done according to FOCUS: depth (cm) depth degradation rate correction factor 0-30 1 30-60 0.5 60-100 0.3 >100 0
36	DSRATE	Adsorbed phase pesticide degradation rate constant (d^{-1})	Same value as for DWRATE. Same correction with depth.
36	DGRATE	Vapour phase pesticide degradation rate constant (d^{-1})	Set to 0 in accordance with FOCUSsw.
37	DPN	Thickness of numerical compartments in the horizon (cm)	Set to 0.1 for 0-10 cm depth and to 5 for depths > 10 cm, in accordance with FOCUSsw.
37	THEFC	Field capacity water content in the horizon ($cm^3\ cm^{-3}$)	Based on pedotransfer functions for water content in the PRZM Manual corresponding to pF 2.5 (FC) and pF 4.2 (WP). The formulae used here additionally ensure that WP < FC and FC < PV, and they account for the presence of stones: $FC = MIN\ [(0.3486 - 0.0018\ SAND + 0.0039\ CLAY + 0.0228\ OM - 0.0738\ BD) * (1\text{-}FSTONES);\ PV - 0.002]$ $WP = MIN\ [(0.0854 - 0.0004\ SAND + 0.0044\ CLAY + 0.0122\ OM - 0.0182\ BD) * (1\text{-}FSTONES);\ FC - 0.01]$ with SAND = sand content (% of mineral component of fine earth) CLAY = clay content (% of mineral component of fine earth) OM = organic matter content (% of fine earth) BD = bulk density (kg/dm3); only refers to fine earth (< 2 mm) FSTONES = volumetric fraction of stones = Vstones/Vtot PV = pore volume fraction = Vpores / Vtot (dm3/dm3)
37	THEWP	Wilting point water content in the horizon ($cm^3\ cm^{-3}$)	

			PV in turn is calculated as: PV = [1 - (fOM * BD)/rhoOM - (1 - fOM) * BD/rhoMin] * (1 - FSTONES) fOM = gravimetric organic matter content, expressed as a fraction (kg/kg) rhoOM = substance density of organic matter (kg/dm3); assumed as 1.1 g cm^{-3} rhoMin = substance density of mineral soil components (kg/dm3), assumed as 2.65 g cm^{-3}
37	OC	Organic carbon content in the horizon (mass-%)	FST- and horizon-specific.
37	KD	Freundlich adsorption coefficient Kf (L kg^{-1})	FST-, horizon- and pesticide-specifc. Calculated as KD = K_{oc} * OC/100.
38	SPT	Initial temperature of the horizon (°C)	Set to BBT in accordance with FOCUSsw. This can be done because we have 6 warmup years.
38	SAND	Sand content (%)	FST- and horizon-specific.
38	CLAY	Clay content (%)	FST- and horizon-specific.
38	THCOND	Thermal conductivity of the horizon	Set to 0 in accordance with FOCUS (parameter not used if IDFLAG = 1)
38	VHTCAP	Heat capacity per unit volume of the soil horizon	Set to 0 in accordance with FOCUS (parameter not used if IDFLAG = 1)
40	ILP	Flag for initial pesticide concentrations in soil before start of simulation	Set to 0 in accordance with FOCUS (no initial pesticide concentration in soil profile).
Record 42 controls the .out output file, which is however not further used in FOOTPRINT. It's only generated for control purposes.			
42	ITEM1	Hydrologic hardcopy	Insert WATR (water variables are output)

		output flag	
42	STEP1	Time step of hydrologic output	Insert YEAR (yearly output)
42	LFREQ1	Frequency of hydrologic output given by a specific compartment number	Set to 5.
42	ITEM2	Pesticide flux output flag	Insert PEST (pesticide flux variables are output)
42	STEP2	Time step of pesticide flux output	Insert YEAR (yearly output)
42	LFREQ2	Frequency of pesticide flux output given by a specific compartment number	Set to 5.
42	ITEM3	Pesticide concen-tration output flag	Insert CONC (pesticide concentration variables are output)
42	STEP3	Time step of pesticide concen-tration output	Insert YEAR (yearly output)
42	LFREQ3	Frequency of pesticide concen-tration output given by a specific compartment number	Set to 5.

42	EXMFLG	Flag for reporting output to file for EXAMS model	Set to 0 (no output to EXAMS).
Records 45 and 46 control the .zts output file, whose content is used and further processed in FOOTPRINT. While record 45 specifies the number of output variables for which time series are to be plotted and the time step, record 46 contains plotting instructions and conversion factors for output to the zts file.			
45	NPLOTS	Number of time series plots (max = 12)	Set to 6 (6 output time series)
45	STEP4	Output time step	Set to DAY (daily output)
46	PLNAME	Name of plotting variable	PLNAME: The following output variables are chosen: 1. RUNF (surface runoff flux) 2. ESLS (eroded soil lost from field) 3. PRCP (precipitation) 4. TETD (total daily evapotranspiration) [only for control purposes] 5. RFLX1 (pesticide surface runoff flux) 6. EFLX1 (pesticide erosion flux)
46	INDX	Index to identify which pesticide if applicable	Set to 1 (there is only one pesticide).
46	MODE	Plotting mode: TSER, TCUM, TAVE, TSUM	Set to TSER (= daily time series) for all output variables
46	IARG	Argument value for PLNAME	Set to 0 (no arguments needed for the chosen output variables).
46	IARG2	Argument value for PLNAME	Set to 0 (no arguments needed for the chosen output variables).
46	CONST	Constant with which to multiply for	CONST: The same conversion factors and thus output units as in FOCUSsw are used. 1. RUNF: use conv. factor of 10 to convert cm to mm

		conversion.	2. ESLS: use conv. factor of 1000 to convert tonne to kg 3. PRCP: use conv. factor of 10 to convert cm to mm 4. TETD: use conv. factor of 10 to convert cm to mm 5. RFLX1: use conv. factor of 10^7 to convert g cm^{-2} to mg m^{-2} 6. EFLX1: use conv. factor of 10^7 to convert g cm^{-2} to mg m^{-2}
			Record 46 finally looks this way: RUNF TSER 0 0 10.0 ESLS TSER 0 0 1.E3 PRCP TSER 0 0 10.0 TETD TSER 0 0 10.0 RFLX1 TSER 0 0 1.E7 EFLX1 TSER 0 0 1.E7

Table 13 - Parameterisation methodology for the PRZM .inp files in FOOTPRINT

4 RUNNING THE MODELS MILLIONS OF TIMES

4.1 Automatic generation of input files for MACRO

The generation of input files was automated and encapsulated in an executable file written in Visual Basic.

4.2 Automatic generation of input files for PRZM

The FOOTPRINT work involves the running of the two pesticide fate models PRZM and MACRO for several millions of time. PRZM modelling tasks were therefore fully automated. These comprised the preparation and formatting of PRZM input files, the running of the model, the extraction of statistics of interest and the archiving of model output files. Full automation was achieved through a combination of macros written in Visual Basic and scripts written in Perl. A total of 3 automation modes were developed: 1) One-at-a-time; 2) Generation of input files; and, iii) Batch mode.

In the one-at-a-time mode, MS Excel is used to create two text files (master.txt and master2.txt) containing a unordered list of all PRZM input parameters and the associated values for a given combination of climate, soil, crop, application date, Koc and DT50. A perl script is then used to read the parameter values listed in the two text files and prepare the .inp and .run input files according to the PRZM formatting requirements. The one-at-a-time also allows the PRZM output files to be post-processed automatically to derive meaningful statistics. The one-at-a-time mode which is controlled through an interface in MS Excel is designed to allow the preparation of PRZM input files, to run the model and to extract model output information for one run only. It is used by FOOTPRINT modellers to evaluate the fate of specific pesticides in specific scenarios and to check results coming out of complex perl scripts. In the Generation of input files mode, the user is invited to list the combinations of climate, soil and crop he is interested in. A loop goes through the various combinations listed and uses the one-at-a-time automation routines described above (combinations of VB and perl scripts) to generate series of 1404 input files for each combination of climate, soil and crop. The 1404 input files cover all combinations of Koc, DT50 and application dates listed in the FOOTPRINT database. The 1404 files are finally compressed together in a rar file which takes the name of the climate, soil and crop combination. The generation of input files mode is used by FOOTPRINT modellers to prepare a large number of input files to be run on the FOOTPRINT@work distributed system. In the batch mode, the user is invited to list the combinations of climate, soil, crop, application date, Koc and DT50 he is interested in. A loop will go through the combinations listed, generate all relevant input files, run PRZM repeatedly and then postprocess results for all the output files created by the model. The batch mode is use by FOOTPRINT modellers to undertake a limited number of automated runs.

5 FROM MODEL PREDICTIONS TO INDICATORS USED IN THE TOOLS

5.1 Summary

The pesticide losses from treated fields predicted by the models MACRO and PRZM have to be converted into actual inputs into surface water and groundwater, taking into account possible risk reduction measures. Subsequently, Predicted Environmental Concentrations (PEC) have to be calculated for groundwater and surface water. These concentrations can subsequently be compared to legal or ecotoxicological thresholds.

In the three FOOT tools, pesticide concentrations in water resources are calculated from simulated pesticide inputs by diffuse sources (drift, surface runoff and erosion, lateral subsurface flow, and tile drainage for surface water; leaching for gorundwater).

For calculation of pesticide inputs into surface water, in FOOT-CRS the real surface water network is used. PECsw are calculated at the catchment outlet (i.e. for one point in space). In contrast, in FOOT-NES and FOOT-FS, hypothetical edge-of-field water bodies adapted from FOCUS (2001) are used. PECsw and PECsed are calculated for each agro-environmental scenario, and afterwards spatially aggregated for display as map or as spatial cumulative distribution function (CDF). PECsw are calculated separately for each input path (surface runoff + erosion + interflow; drainage; drift). In FOOT-NES and FOOT-FS also Predicted Environmental Concentrations in sediment (PECsed) and Time-Weighted Average Concentrations (TWACsw, TWACsed) are calculated.

In FOOT-FS, the risk posed by a pesticide to the aquatic community is assessed by comparing predicted concentrations in surface water with the aquatic ecotoxicological endpoints for the taxonomic groups used as test organisms in the registration procedure (fish, invertebrates, sediment dwelling organisms, higher aquatic plants and algae) using the FOOTPRINT Pesticide Properties Database (PPDB), which is included in the FOOT tools. A simple toxicity/exposure ratio (TER) approach is used for this risk assessment; however, the user is able to view the PEC/TWAC calculated in FOOT-FS and use them to perform a more sophisticated ecological risk assessment (e.g., using mesososm data or Species Sensitivity Distributions SSD) outside the FOOT tools. In FOOT-NES and FOOT-CRS, the user can obtain the (spatial or temporal, respectively) exceedance frequency of user-defined concentration thresholds from the PEC Cumulative Distribution Functions produced by the tools.

For groundwater, the same PEC calculation approach is used in all three tools. PECgw are calculated for the bottom of the soil profile (2 m or shallower, in the presence of impermeable bedrock), not for 1 m depth. Afterwards a qualitative risk assessment for the deeper groundwater can be performed in FOOT-CRS and FOOT-NES by intersecting the obtained PECgw map with the FOOTPRINT SUGAR map. More details can be found in DL23 (Reichenberger et al., 2008b)

5.2 Processing and storage of MACRO and PRZM output in Modelling Databases

From the MACRO and PRZM simulations, 20-year daily time series for pesticide losses (incl. the corresponding water volumes and eroded sediment yield) are available for:

- leaching beyond the lower boundary of the profile (MACRO)
- drainage (MACRO)
- surface runoff (infiltration excess + saturation excess runoff) (PRZM)
- erosion (PRZM)
- lateral subsurface flow (MACRO) (in practice this is also output as drainflow)

Since the time series themselves cannot be distributed with the software due to storage issues, meaningful summary statistics had to be derived and provided with the tools. Selected results (Table 14) from the 20-year simulation time series were then formatted into look-up tables and stored in a large number of MS Access databases (“modelling databases”). When assessments are run in the FOOT tools, data are retrieved from the database based on the relevant climate/soil/crop combinations, the selected percentiles (for FOOT-NES and FOOT-FS), the application months, and K_{oc} and DT50 of the pesticide being modelled.

<table>
<tr><td></td><td>Leaching</td><td>Drainage</td><td>Runoff</td><td>Erosion</td></tr>
<tr><td>FOOT-FS</td><td rowspan="3">Extracted model output: average leaching concentration over the 20-year simulation period; flux concentrations for most soils, resident concentrations for soils with shallow groundwater, no output for soils with impermeable substrate</td><td colspan="3">(same as in FOOT-NES)</td></tr>
<tr><td>FOOT-CRS</td><td colspan="3">Extracted model output: maximum daily loss for each simulation month (n = 240)</td></tr>
<tr><td>FOOT-NES</td><td colspan="3">Extracted model output: percentiles of the whole time series (return period in parentheses):
90th (10 days)
95th (20 days)
96.66th (30 days)
98.0th (50 days),
98.67th (75 days)
99.0th (100 days)
99.33th (150 days)
99.49th (200 days)
99.73th (1 year)
99.90th (about 3 years; though already very uncertain)
99.97th (about 10 years; very uncertain)
→ 11 figures
We store percentiles of the whole 20 year MACRO/PRZM time series rather than annual maxima here, because from an ecological point of view, it is more important to have information also on surface water concentrations with shorter return periods (e.g. with respect to recovery and chronic toxicity) than to have a distribution of annual maximum PECsw.</td></tr>
</table>

Table 14 -Model output values to be stored in the modelling databases

5.3 Groundwater exposure assessment

5.3.1 Accounting for different lower boundary conditions

There are three different cases and thus meanings of pesticide leaching concentration in the modelling databases, depending on the FOOTPRINT hydrologic group FHG (cf. chapter 3, section 2.3):

a) water can percolate through lower boundary of profile → average flux concentration (= total leached mass in 20 years / total percolation in 20 years) is calculated. (FOOTPRINT hydrologic groups L, M, N, W, X, Y)

b) shallow groundwater → zero flux boundary condition in MACRO → no percolation → average resident concentration (arithmetic mean of the 7305 daily resident concentrations in the lowest numerical layer) is calculated (FOOTPRINT hydrologic groups O, P, Q)

c) impermeable substrate → zero flux boundary condition → no percolation → no leaching concentrations is simulated and “-99” is entered in the database (FOOTPRINT hydrologic groups R, S, T, U, V)

These 3 cases (“leaching concentration types”) are considered and treated separately in the FOOT tools. Also the spatial aggregation (cf. section 5.3.2 of this chapter) is done separately for each “leaching concentration type”.

5.3.2 Spatial aggregation of PECgw

While in FOOT-FS the assessment is done for single fields and no spatial aggregation is needed, in the two GIS-based tools FOOT-CRS and FOOT-NES the PECgw are spatially aggregated to polygons for map display and over certain user-selected areas (e.g. administrative units) for display as spatial CDFs.

In FOOT-NES and FOOT-CRS, there are four different options for PECgw aggregation to polygons for map display:

a) area-weighted mean PECgw, referring to only the treated area
b) area-weighted mean PECgw, referring to the total polygon (unique NUTS2/climate/SMU/CLC combination) area
c) flux– and area-weighted mean PECgw, referring to the total polygon area
d) maximum PEC occurring in the treated area (i.e. the highest PEC of all agro-environmental scenarios occurring in the NUTS/climate/SMU/CLC combination)

Note that in all options, “treated area” and “total area” refer to those areas covered with soil typological units (STUs) with the leaching concentration type (flux concentration, resident concentration, no leaching) of concern

While in option c) it is implicitly assumed that groundwater is horizontally well mixed over the polygon area, in the other options it is implicitly assumed that groundwater is not well mixed horizontally.

There are also different options available for the calculation of spatial CDFs of PECgw. First, the user can choose the level of aggregation for which the CDF shall be calculated: i) the whole area of interest, ii) higher-level administrative units (e.g. NUTS0), or iii) lower-level administrative units (e.g. NUTS2 or municipalities). In FOOT-CRS, where the area of interest is a single catchment, only options i) and iii) are available. Then, the user has to choose the statistical population of the CDF:

a) the statistical population of the CDF is the total area of the crop groups (e.g. barley, grain maize, soft wheat) for which applications have been defined in the unit over which the aggregation is performed (AOI, NUTS2, NUTS0)

b) the statistical population of the CDF is only the treated area fraction of the crop groups (e.g. barley, grain maize, soft wheat) for which applications have been defined in the unit over which the aggregation is performed (AOI, NUTS2, NUTS0)

The two different options can lead to quite different CDFs: option a) will yield a vertically narrower CDF with a positive intercept (since non-treated areas have a PECgw of zero). However, the curvature of the CDFs will be the same.

For more details on the spatial aggregation procedures, the reader is referred to DL23 (Reichenberger et al., 2008b).

5.3.3 Dealing with multiple applications

The FOOTPRINT tools offer the possibility of multiple applications, i.e. it is possible that a pesticide is applied within the same polygon (FOOT-CRS and FOOT-NES) or the same field (FOOT-FS) to the same crop more than once, either in different months or even in the same month. Multiple applications to the same area cannot be treated independently of each other, though, because one field treated with one compound can only have one PECgw, and because actual concentrations would be underestimated if the additive effects of multiple applications were ignored. Moreover, in the process of spatial aggregation in FOOT-CRS and FOOT-NES, it has to be avoided that areas are double-counted.

In the FOOT tools, multiple applications (i.e. applications on the same polygon/field in different months, for instance on winter cereals in both April and November, or even in the same month, are handled in the following way for leaching assessments:

- The loads and thus the PECgw from the different applications are simply added up (adding up PECgw is possible because the percolation volume is always the same for the same NUTS2/climate/SMU/CLC/STU/cropID combination in FOOT-CRS/-NES and for the same field in FOOT-FS). This method implicitly assumes that the pesticide molecules from the different applications do not significantly interfere by changing concentration gradients between the micropore and macropore domain compared to a single application.
- In the two GIS-based tools, it has additionally to be taken into account that within a polygon, the treated area fraction can differ between the different applications (cf. next

section). To ensure correct PECgw maps and CDFs, a relatively complex tabular procedure has been put in place (cf. DL23, section 3.1.2.2)

5.3.4 Producing a groundwater risk map

For groundwater risk assessment, FOOT-NES and FOOT-CRS produce, in addition to PECgw maps and CDFs, also a colour-coded “groundwater risk map”. This map contains two variables in its attribute table:

- Risk class (values from 1 to 5) for soils with PECgw as flux concentration (leaching concentration type 1)
- Risk class (values from 1 to 5) for soils with PECgw as resident concentration (leaching concentration type 2)

The map is obtained by intersecting the calculated PECgw map with the FOOTPRINT SUGAR map and assigning risk class values to each resulting polygon according to two matrices of PECgw and SUGAR classes (Tables 15 and 16). Afterwards, a DISSOLVE operation is performed in ArcGIS with the two risk class columns to keep the number of polygons and the file size of the GW risk shape reasonable.

	PECgw of the polygon as calculated by FOOT-NES/-CRS (µg L^{-1})					
SUGAR	<0.001	0.001 to 0.01	0.01 to 0.1	0.1 to 1	1 to 10	>10
<33 (infiltration areas)	2	3	4	4	5	5
33-66	1	2	3	4	4	5
>66 (discharge to SW areas)	1	2	2	3	4	4
1 = very low risk						
2 = low risk						
3 = moderate risk						
4 = high risk						
5 = very high risk						

Table 15 -Relative risk classes for groundwater as a function of PECgw and the SUGAR index

PECgw: 20-year average flux concentration at the lower boundary of the soil profile.
FOOTPRINT soil types with a zero flux boundary condition are exempt from this scheme.

The reasoning for the matrix in Table 15 is that the PECgw at the bottom of the soil profile is not equivalent to the concentration in deeper groundwater. The matrix in Table 15 gives a higher risk class for higher recharge proportion (as estimated with SUGAR) with the same PECgw class. Hence, it considers also the probability that pesticides leached beyond the profile reach the aquifer system.

	PECgw of the polygon calculated by FOOT-NES/-CRS (µg L^{-1})					
SUGAR	<0.001	0.001 to 0.01	0.01 to 0.1	0.1 to 1	1 to 10	>10
<33 (infiltration areas)	1	2	3	3	4	5
33-66	1	1	2	3	3	4
>66 (discharge to SW areas)	1	1	1	2	3	3
1 = very low risk for groundwater						
2 = low risk						
3 = moderate risk						
4 = high risk						
5 = very high risk						

Table 16 -Relative risk classes ("MACRO/SUGAR index") for groundwater as a function of PECgw (resident concentration) and the SUGAR index

PECgw: X^{th} percentile of annual average resident concentration at the lower boundary of the soil profile, for soils with a zero flux boundary condition and shallow groundwater. Note that higher PECgw in these soils can constitute a risk for **surface water** due to lateral flow of shallow groundwater into surface water bodies.

Table 16 applies to the FOOTPRINT soil types with leaching concentration type 2, i.e. shallow groundwater in the profile and permeable substrates (FHG O, P and Q). Because of the shallow groundwater, the lower boundary condition in MACRO has to be "zero flux". Hence, zero percolation will be simulated, and no PECgw as average flux concentration over the full 20 year period (flux concentration = pesticide leaching flux / percolation volume) can be calculated. However, the resident pesticide concentration in the bottom layer (resident concentration = pesticide mass in layer / water volume in layer) is of interest, because groundwater abstraction for drinking water is possible. For these soils, the PECgw represent the long-term average (resident) concentration in shallow groundwater predicted at 2 m depth below the treated field. Concentrations in deeper groundwater and in abstraction wells may be significantly smaller due to attenuation processes such as predominantly shallow lateral groundwater flows to surface water, dilution and degradation. For these reasons, the risk classification system in Table 16 is slightly different from the one in Table 15. However, higher PECgw in these soils can constitute a risk for surface water due to lateral flow of shallow groundwater into surface water bodies.

The FOOTPRINT hydrologic groups R, S, T, U, V have impermeable substrate (which implies zero percolation) and no connection to groundwater. For these hydrological groupings (leaching concentration type 0), risk to groundwater is always very low, and no GW risk map is produced.

5.4 Surface water exposure assessment

5.4.1 General surface water exposure scenario

FOOT-NES: Hypothetical surface water bodies

In comparison to FOOT-CRS, the scale of the assessment is much larger for FOOT-NES (country or EU vs. catchment). Since it is not possible to perform a full-blown landscape analysis and routing of surface runoff in sufficient resolution for a whole country or even the whole of Europe, we follow a water body scenario approach in FOOT-NES. Hypothetical surface water bodies were taken and slightly adapted from the FOCUS surface water scenarios (FOCUS, 2001). In the following, the characteristics of the three surface water body types are described. For the standard case, the FOCUS dimensions for each water body type are adopted (Table 17). However, the FOOT-NES user is able to modify the water body dimensions (except length) in the FOOT-NES Data Manager. All three water bodies, pond, ditch and stream, have a rectangular internal cross-section (vertical side slope).

Type of water body	Width (m)	Total length (m)	Distance from top of bank to water (m)	Minimum water depth (m)
Ditch	1	100	0.5	0.3
Stream	1	100	1.0	0.3
Pond	30	30	3.0	1

Table 17 -Standard dimensions of FOOT-NES water body types (adopted from FOCUS, 2001)

Sediment properties (Table 18) are also adopted from FOCUSsw. Since the STEPS-1-2-3-4 tool (Klein, 2007a), whose STEP-3 equations are used for PECsw and PECsed calculations in FOOT-NES, does not consider suspended solids, suspended solids are not included in the definition of FOOTPRINT water bodies either.

Characteristic	**Value**
Sediment layer depth (cm)	5
Organic carbon content (%)	5 (approx. 9% organic matter)
Dry bulk density (kg m^{-3})	800
Porosity (%)	60

Table 18 -Sediment properties of all FOOT-NES and FOOT-FS water bodies (adopted from FOCUS, 2001)

The user has the possibility to make changes to the following variables:

- water body width (m)
- minimum water depth (m)
- horizontal distance from top of bank to water surface (m)
- total depth of sediment (m)
- gravimetric organic carbon content (fraction)
- sediment dry bulk density (kg dm^{-3})
- sediment porosity (dm^{-3} dm^{-3})

For all three water body types, there is a month-specific, pesticide-free baseflow, calculated as the product of the BFI (baseflow index; available for each FOOTPRINT soil type (FST), the area-specific discharge (available as monthly means for a 30’ × 30’ grid (Fekete et al., 2000; the mean value is already attached to each polygon, i.e. NUTS2/climate/SMU/CLC combination) and the catchment area of each water body.

The concept of an adjacent field and an upstream catchment (Fig.14) has in general been adopted from the FOCUS surface water scenarios. However, there are some modifications to the FOCUS concept (FOCUS, 2001) which are explained in the following:

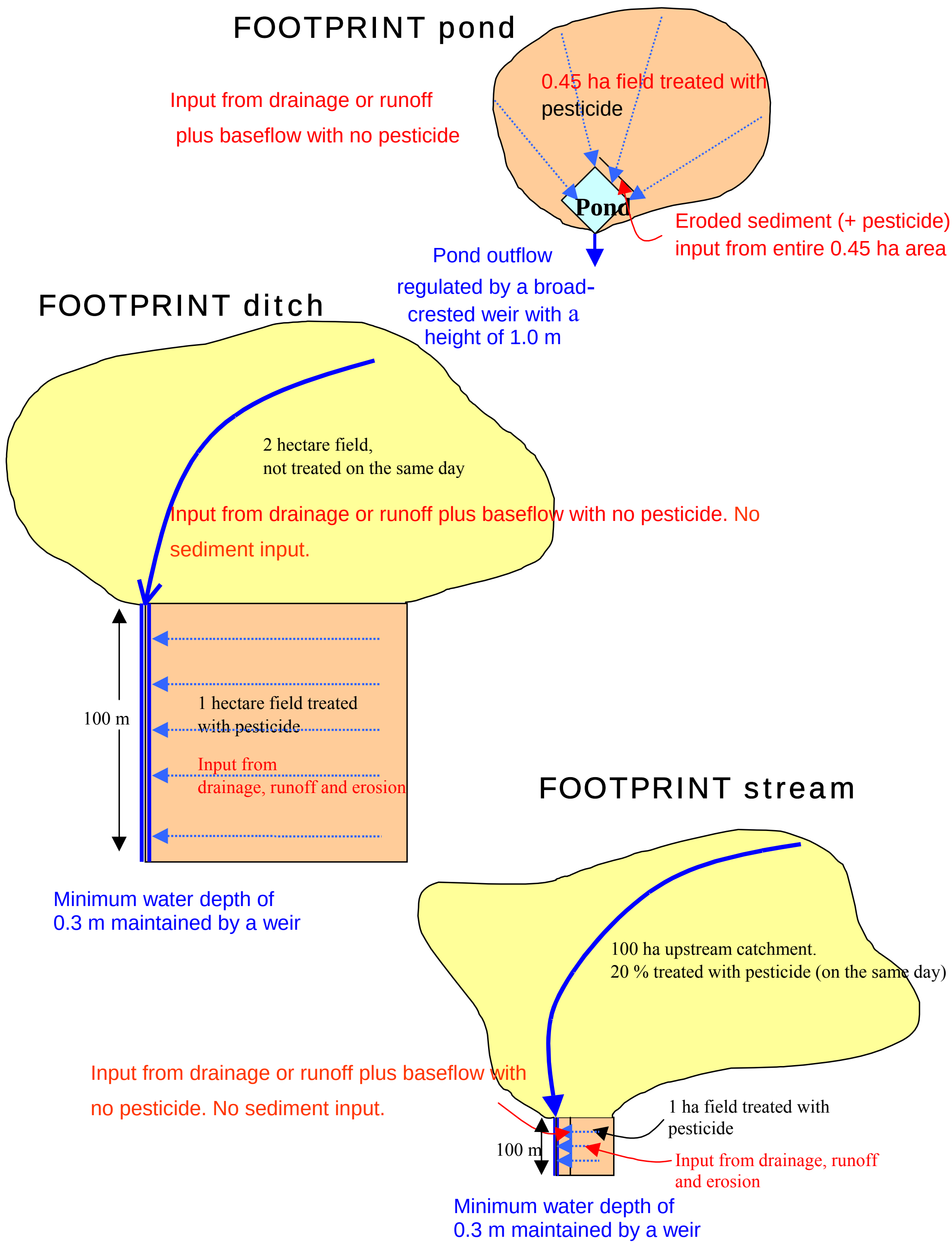


Figure 14 - Conceptual outline of the FOOT-NES and FOOT-FS water bodies (adapted from FOCUS (2001)).

- In FOOTPRINT, *all three* defined water body types (ditch, stream and pond) have an adjacent field that contributes drainage or runoff + eroded sediment (+ lateral subsurface flow, where applicable) fluxes to the water body.
- In addition, also the upstream catchment of the ditch scenario can contribute surface and subsurface runoff to the water body.
- For runoff scenarios, FOCUSsw employed a 20 m 'corridor' adjacent to the pond or stream that contributes eroded sediment and associated pesticides to the pond or stream, with the argument that eroded sediment tends to re-deposit when transported over extended distances. However, the MUSLE and MUSS equations already include deposition (in contrast to the original USLE), because they have been obtained by regression against actual sediment loads at catchment outlets (Williams, 1975). Additionally accounting for sediment deposition is therefore conceptually wrong. *As a consequence, in FOOTPRINT the whole adjacent field contributes eroded sediment and associated pesticides to the water body.*
- While in FOCUSsw, PECsw and PECsed are calculated for simultaneous occurrences of (drift + drainflow) or (drift + runoff + erosion), in FOOT-NES and FOOT-FS PECsw are calculated separately for i) drift, ii) runoff + erosion (+lateral subsurface flow), and iii) drainflow, because we judged it not realistic that higher percentile events with a return period of several months of runoff/erosion or drainage inputs coincide with each other or a pesticide application day. Moreover, the influence of each input pathway on concentrations in surface waters becomes visible this way.

The following settings have been adopted from FOCUS without change:

- The fraction of the upstream catchment that is treated *on the same day* with pesticide as the adjacent field is 0 % for the ditch and 20 % of the stream. This percentage is not to be confused with the percentage of the crop that is treated at all (which is entered in the Pesticide Scenario Manager and accounted for *after* the PECsw calculation for a single scenario combination).
- No eroded soil or associated pesticide is received from the upstream catchment as all such soil is assumed to be incorporated within the upstream water body. (If the FOOT tool evaluation reveals that this yields too low estimates for erosion, this setting may be removed so that also the upstream catchment contributes eroded sediment).

In the MUSS equation, there is a slight positive correlation of area-specific sediment yield with the contributing area and a slightly negative correlation with the hydraulic length

(Carsel et al., 2003). Because these effects are only slight and also counteracting, it was deemed justifiable to use the same PRZM modelling runs (calculated for a 1 ha square field with 118.8 m hydraulic length) also for the 0.45 ha catchment of the pond.

The areas contributing pesticide inputs to the different water bodies in FOOTPRINT are summarized in Table 19.

Water Body	**Drift, drainage or surface runoff pesticide fluxes (dissolved) contributed from:**	**Pesticide fluxes associated with eroded sediment (adsorbed) contributed from:**
Pond	All the 0.45 ha catchment.	*All the 0.45 ha catchment*
Ditch	The adjacent 1 ha field only.	*The adjacent 1 ha field.*
Stream	The adjacent 1 ha field plus 20 ha of the upstream catchment.	*The adjacent 1 ha field.* (None from the upstream catchment)

Table 19 -Areas contributing pesticide inputs (dissolved and adsorbed) to the different water bodies inFOOT-NES and FOOT-FS. Differences to FOCUSsw are highlighted in italics.

It has to be noted that in FOOT-NES and FOOT-FS (as well as in FOCUSsw) it is assumed that the entire catchment of the hypothetical surface water body (adjacent field + upstream catchment) has the same soil type, the same crop type and is subject to the same weather time series.

FOOT-FS: Hypothetical surface water bodies

In the farm-scale tool FOOT-FS, the surface water bodies have the same upstream catchments of ditch and stream as in FOOT-NES, and the same default sediment properties as the FOOT-NES default settings. The sediment properties can be changed by the FOOT-FS user in the Settings menu. The water body dimensions (length, width, depth), size of the adjacent field (for drainage/runoff/erosion) and field length adjacent to the water body (for drift calculations) are always user input.

Again, the fraction of the upstream catchment that is treated *on the same day* with pesticide as the adjacent field is set to 0 % for the ditch and 20 % of the stream.

FOOT-CRS: Observed surface water network

In FOOT-CRS, the real (or rather, an observed) surface water network is used for calculating pesticide inputs into surface water and resulting PEC. Both the surface water network itself (as a polyline shapefile) and the catchment boundaries (as a polygon shapefile) are needed in FOOT-CRS. The default data source is the European River and Catchment Database CCM2 (Vogt et al., 2007a; Vogt et al., 2007b).

5.4.2 Spray drift inputs into surface water

In FOOT-NES and FOOT-FS, PECsw are calculated for hypothetical, edge-of-field water bodies. Since the distance between treated field and bank of the water body is either default or user input, calculations have only to be performed for one direction.

In FOOT-CRS, drift inputs are calculated on a vector basis for each river segment (the surface water network has to be provided in polyline shape format). Here, drift calculations have to be performed for eight possible wind directions (N, NE, E, SE, S, SW, W, NW), and mitigating landscape elements like hedges and riparian vegetation between the water body and treated fields have to be accounted for in the calculations.

The drift loading of a water body (in % of the application rate) is calculated ain all three tools using the drift function proposed by FOCUS (2001) and Rautmann et al. (2001). The parameters of the drift function for the different percentiles (90, 82, 77, 74, 72, 70, 69, 67, 50) have been obtained by fitting the equation to the different empirical percentiles of the BBA drift raw data (Rautmann et al., 2001). While in FOOT-NES and FOOT-CRS the user can choose between different percentiles of the Ganzelmeier/Rautmann drift distribution, in FOOT-FS always the 90th percentile is used.

In FOOT-NES and FOOT-FS, the calculated pesticide drift input feeds into the PECsw/sed calculation routines adopted from the STEP-3 part of the tool STEPS-1-2-3-4 (M. Klein, IME Schmallenberg; Klein, 2007a). In FOOT-CRS, in contrast, inputs are summed up over the catchment area.

5.4.3 Drainage inputs into surface water

There are three different cases and thus meanings of pesticide drainage losses in the metamodel database, depending on the FOOTPRINT hydrological group (cf. chapter 3, section 2.3):

a) the soil is artificially drained → variables in the modelling databases denote actual pesticide drainage loss and corresponding drainflow volume
(FOOTPRINT hydrologic groups Q, U, V, Y)

b) the soil is not artificially drained, but lateral subsurface flow (“interflow”) occurs → variables in the modelling databases denote pesticide loss via subsurface flow and corresponding interflow volume
(FOOTPRINT hydrologic groups O, P, R, S, T, W, X)

c) the soil is neither artificially drained nor does interflow occur → no drainage loss simulated → value "-99" is entered in the database (FOOTPRINT hydrologic groups L, M, N)

These 3 cases ("drainflow types") are considered and treated separately in the FOOT tools. Also the spatial aggregation is done separately for each "drainflow type".

In FOOT-NES and FOOT-FS, the calculated pesticide drainage input feeds into the PECsw/sed calculation routines adopted from the STEP-3 part of the tool STEPS-1-2-3-4 (Klein, 2007a). In FOOT-CRS, in contrast, pesticide drainage inputs and drainflow volumes are summed up over the catchment area.

5.4.4 Surface runoff and erosion inputs into surface water

In FOOT-NES and FOOT-FS, the calculation of pesticide surface runoff and erosion inputs into surface water bodies is straightforward. If no mitigation measures are specified (cf. section, pesticide inputs into surface water are equal to pesticide losses from the field as calculated with PRZM.

In FOOT-CRS, In FOOT-CRS, surface runoff and erosion inputs into surface water are calculated from pesticide losses using a grid-based routing procedure.

In contrast to FOOT-NES and FOOT-FS, the FOOT-CRS modelling databases do not contain 11 pesticide loss percentiles of the whole 20-year time series, values for each of 240 simulation months:

- max. daily pesticide runoff loss (mg m^2 d^{-1})
- associated precipitation (mm d^{-1})
- max. daily pesticide erosion loss (mg m^2 d^-1)

To keep calculation times at an acceptable level, the surface runoff routing for the catchment is not performed for each simulation month, but only 30 times to create the basis for interpolation:

(5 climate-specific standard rainfall volumes * 2 seasonal conditions * 3 different species (surface runoff water, pesticide dissolved in surface runoff, pesticide adsorbed to eroded sediment). Afterwards, the results of the runoff routing are aggregated to polygons (using the zonal statistics functionality of ArcGIS), and a linear interpolation based on precipitation volumes is performed for each polygon of the catchment and each of the 240 simulation months. The following variables are interpolated:

- initial surface runoff volume (mm d^{-1})

- fraction of initial surface runoff volume reaching the sw network
- fraction of pesticide runoff loss reaching the sw network
- fraction of pesticide erosion loss reaching the sw network

The pesticide inputs into the surface water network from each polygon are then obtained by multiplying the pesticide losses with the above-calculated fractions reaching the surface water network.

The basic principles of the surface runoff routing procedure in FOOT-CRS are:

- Standard ArcGIS Spatial Analyst raster functionality is used („flow accumulation", „downstream flow length", etc.)
- Initial surface runoff is calculated with the Curve Number approach (CN have been adjusted to reflect exclusively surface runoff)
- "Infiltration capacity" is given as max[(initial abstraction – precipitation),0] → cells which generate initial surface runoff cannot infiltrate water coming from upslope
- It's assumed that infiltration and sedimentation are the only processes reducing pesticide load in surface runoff
- Outflow of eroded sediment from a cell is reduced by a slope-dependent reduction factor compared to the outflow of surface runoff water
- Wetlands intercept parts of the dissolved and particle-bound pesticide load, but pass on the full water volume to the surface water network

In FOOT-NES and FOOT-FS, the calculated pesticide runoff and erosion inputs feed into the already mentioned STEP-3 PECsw/sed calculation routines. In FOOT-CRS, however, inputs are summed up over the catchment area.

5.4.5 PECsw/sed calculation

In the FOOT tools, loads and PECsw/PECsed are estimated separately for drift, runoff + erosion, and drainage. 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.

Calculation of Predicted Environmental Concentrations in surface water and sediment (PECsw/sed) 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.

STEPS-1-2-3-4 (Klein, 2007a) is an upgrade of the STEPS-1-2-calculator used in the lower tier calculations of the FOCUSsw scenarios (FOCUS, 2001). STEP-3, whose equations are used in FOOT-FS and FOOT-NES, was created as a quick replacement of the very complex and computation-intensive TOXSWA model (FOCUS, 2001). While being much faster, STEP-3 yields almost the same results as TOXSWA (Klein, 2007b). STEP-3 simulates a water-sediment system, with the sediment being split into an upper and a lower layer. It works on an hourly basis and goes through a loop in each simulation hour. Within a loop, STEP-3 sequentially simulates all transport and transformation processes (water inflow, complete mixing of the water column, diffusive exchange between water column and sediment and between the two sediment layers, pesticide sorption and degradation, water outflow).
Within FOOTPRINT, the STEPS-1-2-3-4 calculation is run for 28 consecutive days. On the first day, the pesticide inputs from the MACRO or PRZM metamodel or from the drift calculations are added. The following days are run with zero inputs of pesticide and runoff/drainflow.The STEPS-1-2-3-4 algorithms produce both

a) initial PECsw and PECsed and
b) time weighted average concentrations (TWAC) over user-specified periods from 1 to 28 days.

As explained above, PECsw/PECsed are assessed separately for each pathway (drift, drainage, runoff/erosion). For scenarios where subsurface lateral flow occurs, the X^{th} percentile pesticide loss via subsurface flow calculated with MACRO (i.e. emulated with primary drains) and corresponding flow volume is added to the PECsw calculations for the pathway runoff and erosion.

In FOOT-CRS, which operates at the catchment scale, the aim is concentrations at the outlet, or even exceedance frequencies of x µg L^{-1} (usually 0.1 µg L^{-1}) in a given period. This implies that results must be aggregated meaningfully. The following phenomena become important at the catchment scale:

- 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 during transport in the water course
- spatial and temporal variability of weather and application dates

The standard version of the Gustafson equation (which is used to account for geomorphological dispersion; cf. Gustafson et al., 2004) does not account for sorption and degradation yet. Therefore, pesticide sorption and degradation during transport in the water course are (conservatively) neglected at least in the first version of FOOT-CRS. Interaction between water column and sediment is handled in a strongly simplifying, but conservative way with respect to PECsw:

- The fraction of particle-bound pesticide inputs that is transported downstream from its point of entry is estimated with a simple approach assuming instantaneous sorption equilibrium at the point of entry between the flowing water body and the bed sediment and neglecting sediment pore water. During the downstream transport of this fraction, no more interaction with the bed sediment is considered.
- For pesticide inputs into the water column (drift, drainage, surface runoff, lateral subsurface flow), no interaction with the bed sediment is considered.

For further details on the calculation of PEC in surface water in either FOOT-NES, FOOT-FS and FOOT-CRS, the reader is referred to DL23 (Reichenberger et al., 2008b)

5.4.6 Spatial aggregation of losses, inputs and PEC

In the two GIS-based tools, all output variables (losses, inputs and PEC) except for the PECsw in FOOT-CRS have to be spatially aggregated for display as map or CDF.
In FOOT-NES and FOOT-CRS, there are three different options for PECgw aggregation to polygons for map display:

a) area-weighted mean loss/input/PEC/TWAC, referring to only the treated area
b) area-weighted mean loss/input/PEC/TWAC, referring to the total polygon (unique NUTS2/climate/SMU/CLC combination) area
c) maximum loss/input/PEC/TWAC occurring in the treated area (i.e. the highest loss/input/PEC/TWAC of all agro-environmental scenarios occurring in the NUTS/climate/SMU/CLC combination)

For the input pathway drainage, in all options, “treated area” and “total area” refer to those areas covered with soil typological units (STUs) with the drainflow type (artificial drainage, lateral subsurface flow, neither of them) of concern.
The options for the calculation of spatial CDFs are the same as for groundwater.

5.4.7 Dealing with multiple applications

It is possible that a pesticide is applied within the same polygon to the same crop more than once (either in different months or even in the same month). The problems arising from multiple application differ between the input pathway drift and the soil-related pathways drainage, surface runoff and erosion, and also between inputs into surface water and the resulting PEC.

Spray drift inputs

For the calculation of drift inputs into surface water multiple applications to the same field can be treated independently of each other. When calculating PEC due to drift, however, multiple applications cannot be treated independently any more, because concentrations will be underestimated if at the time of application there are residues from previous application.left in the water/sediment system.

In FOOT-NES, drift inputs resulting from multiple applications (i.e. applications on the same field in different months, for instance on winter cereals in both April and November, or even in the same month) are dealt with as follows:

- For the spatial aggregation, the maximum drift load from the different applications is taken. This is appropriate because the aim of surface water exposure assessment is peak concentrations in water bodies, not average concentrations.
- However, it has additionally to be taken into account that within a polygon, the treated area fraction (Ftreated) can differ between the different applications. To ensure correct maps and CDFs, a relatively complex tabular procedure has been put in place (cf. DL23, section 4.2.1.2.2). This procedure is essentially the same for drift inputs, drainage losses and inputs, runoff and erosion losses and inputs, PECsw/sed and TWACsw/sed.

Drainage, runoff and erosion inputs

In contrast to drift, for the pathways runoff, erosion and drainage input events are triggered by rainfall events, not by pesticide application. If two applications take place in the same calendar month, it can be assumed that the pesticide runoff/erosion or drainage inputs from the two applications occur on the same day. So there is no carryover in water and sediment (because there is only one input event), but there is some carryover in the field from the first application to the second.

In FOOT-NES and FOOT-CRS, pesticide drainage/runoff/erosion inputs resulting from multiple applications (i.e. applications on the same field in different months, for instance on winter cereals in both April and November, or even in the same month) are dealt with as follows:

- If there are two or more applications in different calendar months, they are treated as independent.

- If there are two more applications in the same calendar month, we update the pesticide application rates by calculating the residues from the first application in the field and adding them to the application rate of the second application (the process is repeated for additional applications). In mathematical form:

Be there n applications, application_1 at t_1, application_2 at t_2, application_n at t_n.
For a single application, the residues from that application at time t are obtained as:

residue (t) = application_rate * exp (- ln2/DT50 * t) (18)

For a sequence of applications, it follows:
application_rate_2_updated = application_rate_1 * exp (- ln2/DT50 * (t_2 - t_1)) + application_rate_2 (19)
application_rate_3_updated = application_rate_2_updated * exp (- ln2/DT50 * (t_2 - t_1)) + application_rate_3 (20)
application_rate_n_updated = application_rate_n-1_updated * exp (- ln2/DT50 * (t_n – t_{n-1})) + application_rate_n. (21)

- Then ALL updated application rates (application rate + residues from previous applications) within each calendar month are used together with the metamodel output to calculate drainage losses and inputs.
- Subsequently, in FOOT-NES ALL resulting pesticide inputs into sw within each calendar month are used to run STEPS.
- For the spatial aggregation, the maximum drainage loss/input from the different application is taken. This is appropriate because the aim of surface water exposure assessment is peak concentrations in water bodies, not average concentrations.
- However, it has additionally to be taken into account that within a polygon, the treated area fraction (Ftreated) can differ between the different applications.

In FOOT-FS, there is a slight difference in the methodology. In contrast to FOOT-NES and FOOT-CRS, where applications in different calendar months are treated as independent, in FOOT-FS residues from applications in one calendar month are carried over to applications of the same active in the next month (provided the interval between the last application in one calendar month and the first application in the following month is not longer than 28 days).

Subsequently, the highest updated application rate (application rate + residues from previous applications) within each calendar month is selected and used together with the modelling database output to calculate pesticide losses and inputs and run STEPS.

PECsw/sed in FOOT-NES and FOOT-FS due to drift inputs

When calculating PECsw/sed due to drift, multiple applications cannot be treated independently any more, because concentrations will be underestimated if at the time of application there are residues from previous application.left in the water/sediment system.
In FOOT-NES and FOOT-FS, PECsw/sed,drift resulting from multiple applications are dealt with as follows:

- Each application (active substance) is assessed individually in STEPS. The residues in the water/sediment system from the n^{th} application at the time of the $n+1^{th}$ application following application feed into the STEPS run for the $n+1^{th}$ application. The interval between applications is known because the user also enters the application day in the Pesticide Scenario Manager.
- For the spatial aggregation, the highest PECsw (analogously: PECsed, TWACsw, TWACsed) of the PECsw calculated in the different simulation runs for a particular application month is taken as the final PECsw for this application month ("PECsw,drift,final" in the following). This is appropriate because the aim of surface water exposure assessment is peak concentrations in water bodies, not average concentrations.
- However, it has additionally to be taken into account that within a polygon, the treated area fraction (Ftreated) can differ between the different applications.

PECsw/sed in FOOT-NES and FOOT-FS due to drainage, runoff and erosion inputs

For the input pathways drainage and runoff/erosion, multiple applications in the same calendar month are already dealt with before running STEPS by adjusting the pesticide application rates. Therefore, the PECsw (analogously: PECsed, TWACsw, TWACsed) due to drainage or runoff/erosion inputs calculated with do not need further adjustments. With respect to spatial aggregation, PECsw due to drainage, runoff and erosion inputs can be treated the same way as PECsw due to drift (see above).

5.5 Incorporating the effect of mitigation measures

The following mitigation measures (Table 20) are available in the tools for the user to reduce pesticide inputs into surface water and groundwater. It turns out that a large part of the mitigation measures listed in Table 20 are already implicitly included in the Pesticide Scenario Manager (FOOT-CRS/-NES) or the Pesticide Programme Manager (FOOT-FS), i.e. their effect can be assessed by changing the pesticide application scenario (compound, crop, application rate, application date, percentage treated). Other landscape-independent mitigation measures, like the use of drift-reducing technology, can be directly specified by the user in the tools. With regard to mitigating landscape elements like hedges, riparian buffers, grassed edge-of-field buffers, grassed waterways and constructed wetlands, there is a difference between the three tools:

- In FOOT-FS, these elements are specified by the user for each field
- In FOOT-NES, these elements are specified by the user for each set of selected polygons
- In FOOT-CRS, these elements are fed into the system through a landscape feature shapefile (real, observed elements), a mitigation feature shapefile (hypothetical, user-drawn elements) or the land cover / land use map (if its spatial resolution is good enough).

	List of mitigation measures explicitly or implicitly included in the different tools		
	mitigation measures measures are already implicitly or explicitly included in Pesticide Scenario Manager (FOOT-CRS/-NES) / Pesticide Programme Manager + Scenario Builder (FOOT-FS) effect is directly calculated in the GIS (if spatial resolution of input maps is fine enough) effect is directly calculated in the GIS, but a buffer has to be specified by the user beforehand reflected in the Mitigation Manager as spatially variable mitigation factor reflected in the Mitigation Manager as spatially constant (global) mitigation factor reflected in the FOOT-FS Scenario Builder reflected in the My Equipment section of FOOT-FS included explicitly or implicitly n the FOOT-CRS point source assessment (part of the FOOT-CRS Pesticide Scenario Manager) not considered at this stage (possibly in later versions)		
pathway	**FOOT-FS**	**FOOT-CRS**	**FOOT-NES**
drift	1. reduction of application rate 2. product substitution) 3. minimum distances 4. riparian buffer strips and hedges 5. change crop / land use 6. drift reducing technology (several options) 7. change of application date (matters only for pome/stone fruit)	1. reduction of application rate 2. product substitution 3. minimum distances 4. riparian buffer strips and hedges 5. change crop / land use 6. drift reducing technology (several options) 7. change of application date (matters only for pome/stone fruit)	1. reduction of application rate 2. product substitution 3. minimum distances 4. riparian buffer strips and hedges 5. change crop / land use 6. drift reducing technology (several options) 7. change of application date (matters only for pome/stone fruit)
drainage	1. reduction of application rate 2. product substitution 3. shift of application date? (only monthly shifts lead to a change in results) 4. application restrictions in time and/or space 5. change crop / land use	1. reduction of application rate 2. product substitution 3. shift of application date? (only monthly shifts lead to a change in results) 4. application restrictions in time and/or space 5. change crop / land use	1. reduction of application rate 2. product substitution 3. shift of application date (only monthly shifts lead to a change in results) 4. application restrictions in time and/or space 5. change crop / land use
leaching	1. reduction of application rate 2. product substitution 3. shift of application date (only monthly shifts lead to a change in results) 4. application restrictions in time and/or space 5. change crop / land use	1. reduction of application rate 2. product substitution 3. shift of application date (only monthly shifts lead to a change in results) 4. application restrictions in time and/or space 5. change crop / land use	1. reduction of application rate 2. product substitution? 3. shift of application date (only monthly shifts lead to a change in results) 4. application restrictions in time and/or space 5. change crop / land use
Surface runoff and erosion	1. reduction of application rate 2. grassed edge-of-field buffer strips 3. product substitution 4. riparian buffer strips and hedges 5. shift of application date (only monthly shifts lead to a change in results) 6. application restrictions in time and/or space	1. reduction of application rate 2. grassed edge-of-field buffer strips 3. product substitution 4. riparian buffer strips and hedges 5. shift of application date (only monthly shifts lead to a change in results) 6. application restrictions in time and/or space	1. reduction of application rate 2. grassed edge-of-field buffer strips 3. product substitution 4. riparian buffer strips and hedges 5. shift of application date (only monthly shifts lead to a change in results) 6. application restrictions in time and/or space

	7. change crop / land use 8. grassed waterways 9. constructed wetlands	7. change crop / land use 8. grassed waterways (this is basically a grassed buffer strip in slope direction, usually located where overland flow accumulates (little talwegs on a slope); it's NOT a ditch or other water body) 9. constructed wetlands 10. strip cropping	7. change crop / land use 8. grassed waterways 9. constructed wetlands
Point sources	No calculations, instead FOOT-FS point source audit (cf. section 5.1)	1. mixing pesticides, filling and cleaning sprayers on biobeds or on the field 2. safe storage and disposal of containers 3. no application on the farmyard? 4. Characteristics of farmyards in the catchment (paved, asphalt, dirt, concrete)? 5. Degree of connectedness of farmyards in the catchment to sewer system? 6. sharing spraying equipment or spraying by contractors? 7. regular inspection of sprayers	not applicable

Table 20- List of mitigation measures included in the different tools

5.6 Final output of the three tools

The final output of the exposure assessment in FOOT-NES is, for a given active ingredient:

- Maps and spatial cumulative distribution functions (CDFs) of
  - pesticide leaching concentrations (PECgw)
  - pesticide losses from fields
  - pesticide inputs into surface water
  - Predicted Environmental Concentrations and Time Weighted Average Concentrations in surface water and sediment (PECsw/sed and TWACsw/sed)
- A "groundwater risk map".

The final output of the exposure assessment in FOOT-CRS is, for a given active ingredient:

- Maps and spatial cumulative distribution functions (CDFs) of
  - pesticide leaching concentrations (PECgw)
  - pesticide losses from fields
  - pesticide inputs into the surface water network
- Temporal CDFs of Predicted Environmental Concentrations in surface water (PECsw) at the catchment outlet. From these, exceedance frequencies and return periods of given monthly maximum concentrations can be directly calculated.
- A "groundwater risk map".

The final output of a FOOT-FS exposure and risk assessment is, for a given pesticide programme (which may comprise several products and several active ingredients):

- A single PECgw value for each active ingredient.
- A single PECsw value for each active ingredient and input pathway
- Toxity/Exposure Ratios (TERs) for each combination of active ingredient, input pathway and taxonomic group used for aquatic regulatory assessments (fish – acute, fish – chronic, invertebrates – acute, invertebrates – chronic, higher aquatic plants, algae – acute, algae – chronic). The TERs are simply obtained by dividing an ecotoxicological endpoint of the compound (e.g. EC50 for aquatic invertebrates – acute exposure) by the calculated PECsw.

Since the intended users of FOOT-FS are farmers and extension advisers, which are usually not acquainted with aquatic risk assessment procedures, with the default output settings in FOOT-FS only colour-coded risk bars are presented to the user. However, PECgw, PECsw and TERs can be made visible by using the "advanced" output settings.

6 DISCUSSION AND PERSPECTIVES

The parameterization of MACRO and PRZM, as well as the exposure assessment calculations in the three tools have been described in detail. They include several newly developed and innovative procedures, especially with respect to the MACRO model. Needs for revision may concern the MACRO and PRZM parameterization, but are more likely to involve the exposure assessment methodologies that convert the MACRO and PRZM output to pesticide inputs into surface water and resulting concentrations. Potential fields for further improvements of the tools are, for instance:

- Using a more sophisticated flow accumulation algorithm (e.g. MD∞) for the surface runoff routing in FOOT-CRS instead of the D8 algorithm used by the ArcGIS flow accumulation functionality.
- More sophisticated treatment of in-stream fate processes in FOOT-CRS (for instance, degradation in the river system is not taken into account at the moment)
- Possible replacement of the static Gustafson CDE approach with an actual flow routing in the channel network (e.g. Muskingum routing).
- More sophisticated treatment of mitigation of pesticide runoff and erosion inputs into surface waters by constructed wetlands (in all three tools).

Any future upgrades of exposure assessment methodologies in the three FOOT tools will first be thoroughly tested against experimental data and then be included in updates of the FOOT tools in the course of regular maintenance releases.

CHAPTER 4 – THE FOOTPRINT TOOLS

1 OVERVIEW

1.1 Introduction

The principal aim of the FOOTPRINT project has been to develop computer tools to evaluate and reduce the risk of pesticides impacting on surface and groundwater resources in the EU. The approach was to develop three tools that use the same underlying principles, science and data, but which serve the needs to different user communities at different geographical scales. These scales range from the farm and field scales (FS), to the catchment and regional scales (CRS), to the national and EU scales (NES).

1.2 The FOOT-Tools

1.2.1 FOOT-FS

FOOT-FS has been developed for use at the local level (farm/field scale). The target users are agricultural advisers and farmers, although users can be anyone who wishes to explore scenarios at this level. The main approach of FOOT-FS has been to make a complex issue more 'digestible' by simplifying the assessment and reporting processes. For example, breaking down the data required into reusable blocks of data (to avoid repetitive data input) and the use of graphical displays and icons to convey results. The tool also suggests potential mitigation options allowing users to explore what-if scenarios and is supported with a number of tools and documents to help promote the adoption of good practices.

1.2.2 FOOT-CRS

FOOT-CRS has been designed for scales ranging from small catchments to regional levels. The target users are water managers and include local authorities, environment agencies, water companies or stewardship managers. FOOT-CRS is an add-on to the ESRI ArcGIS software. The tool uses the predictions made by the pesticide fate models for each FOOTPRINT agro-environmental scenario and routes these through the landscape to the nearest point of entry into the surface water system. The transport through the river network is approximated with a simple equation analogous to the convection-dispersion equation (CDE).

1.2.3 FOOT-NES

FOOT-NES has been designed for large-scale studies at national or EU level. The target users are EU/national policy and decision-makers, of environment ministries and agencies. The tool may also be of interest to pesticide registration authorities. FOOT-NES is also an add-on to the ESRI ArcGIS software. FOOT-NES aims to identify those large areas which are most at risk of pesticide contamination and to assess the probability of pesticide concentrations exceeding legal or ecotoxicologically-based thresholds at the member state and EU levels.

2 FOOT-FS

2.1 Introduction

2.1.1 Development tools

FOOT-FS has been developed using Microsoft (MS) Visual Basic 6.0 to create the graphical user interface and calculation routines. MS Access is used to store data. The multi-language capability has been created using a Visual Basic 6 add-on developed by Softwarebuero Jollans (http://jollans.com). The user does not require any software to be installed in order run FOOT-FS - they only need to run the FOOT-FS installation routine. The FOOT-FS installer has been created using MS Visual Studio Installer 1.1.

2.1.2 FOOT-FS Overview

FOOT-FS is the FOOTPRINT farm-scale tool and is mainly intended for use by extension advisers, farmers, agronomists and others interested in evaluating risks at the field level. 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 for best practice and mitigation options to limit transfers of pesticides in the local agricultural landscape.

The software is a collection of modules and tools that can be used independently of each other, but usually they are collectively managed from within a simple software shell (the FOOT-FS shell) that is driven by a series of navigation menus. This approach breaks the modelling and risk assessment process down into a number of discrete steps thus making it easier to use.

2.1.3 Multiple languages

The FOOT-FS software will be available in 8 languages: English, French, German, Greek, Italian, Polish, Slovenian and Swedish. Translation into different languages has presented a number of problems to overcome. This includes translating some often technical and specific terms, designing the user interface to cope with variable length of text and coding the software to cope with different language character sets and use of different symbols.

2.2 FOOT-FS Shell

The FOOT-FS Shell provides access to all the FOOT-FS modules and facilities and runs the risk assessment and reporting routines. There are three main sections in the shell:

My Data: Facilities to collate, check, format and store data provided by the user, which is then used to drive the risk assessments.

FOOT-FS Assessments: Routines to run the assessment and then deliver the results to the user in an appropriate format.

Toolbox: A collection of tools that are designed to help the user get the most out of the software and which extend and enhance its functionality.

2.3 My Data

The My Data section of the shell provides access to a number of tools to build up reusable blocks of data that can be used to construct FOOT-FS risk assessments. The tools include:

- Scenario Builder
- Pesticide Programme Builder
- My Equipment
- Data Manager

2.3.1 Scenario Builder

The Scenario Builder provides the user with a facility to build up a collection of farms and fields and record information about each field including:

- The crop being grown and the field size
- The soil type

- The climate zone
- Field features (hedgerows/buffer vegetation, water bodies, etc.)

The Scenario Builder also has a data checker to ensure the user makes valid selections.

Crop and field size

This facility allows the user to select a crop from the list of about 80 crops. As a crop is selected the relevant Footprint crop type (the crop type to be used for modelling purposes) is allocated. In this tool each crop also has an associated picture of the crop to aid with crop selection across Europe (where common names could differ and thus cause confusion). The user also enters the size of the field when they select the crop.

Soil type

The FOOTPRINT Soil Type Selector provides an electronic form of a complex questionnaire / flowchart which guides the user through to selecting one of over potentially 900 FOOTPRINT soil types (FSTs). This process has been streamlined and is completed via a maximum of 7 questions. The soil selection process also identifies the Flow Pathway Category (FPC). (See Deliverable DL8)

There is also the option to access definitions, a glossary and further information about some of the scientific terms used within the questionnaire.

Climate zone

Selection of the Climate Zone is achieved via a ‘clickable’ map of Europe showing the 16 Footprint climate zones (FCZs) (see Deliverable DL9). The user simply clicks on the map with his/her mouse and details regarding the climate zone are displayed on the left. The FCZ can then be selected as required.

Field features

Data on the features in the field and the field margin are entered in order to calculate potential mitigation options. This includes features such as constructed wetlands, grassed waterways, grass strips, hedgerows and details of any water bodies adjacent to the field. The screen has a pictorial layout to aid the user in identifying the data required.

Data on hedgerows/buffer vegetation is required in order to assess the risks from spray drift and for evaluating potential mitigation options. A facility to enter details about any hedgerows that exist between the field and any water bodies adjacent to the field (see below) is provided within FOOT-FS. The details of the hedgerow include whether it is deciduous or evergreen and its width (2-20 m).

Details of any surface water bodies are also required by the calculation routines. A graphical facility is provided allowing the user to enter details of surface water bodies close to the field being evaluated. Data required includes:

- Water body type – stream, ditch, pond etc.
- Physical dimensions – width, depth etc.

Data checker

The number of possible combinations of crop, climate zone and soil type are vast and thus not all of the possible combinations have been modelled. In order to ensure that the user selects an appropriate combination the Scenario Builder has a data checker facility. This facility performs a number of functions. Firstly it checks that all required data for a particular field have been entered. Secondly it checks to see if the combinations selected have actually been modelled (and thus the user can run an assessment). Thirdly, it checks to see if the user has the relevant results databases downloaded and installed, thus highlighting to the user if they need to use the Results Database Download Tool (see below) to obtain the relevant data to run an assessment.

2.3.2 Pesticide Programme Builder

The Pesticide Programme Builder allows the user to create a list of pesticides that are to be applied to a field. The programme consists of:

- The product applied
- The date of application
- The rate of application (kg or l/ha)

To support the process the user can set up a number of pesticide product ‘brands’. Each brand consists of:

- A distinctive name e.g. the brand name
- The active substances the brand contains
- The proportion of those active substances in the product (g/l or % w/w)
- The typical application rate.

Thus when a user is creating a pesticide programme, as he/she selects the product/brand all the details about the active substances and amounts are transferred in the programme without the user having to re-enter them - they only need to adjust the application rate if required.
Once a user has created a pesticide programme it can be copied, deleted or amended - allowing the user to rapidly build-up variations of programmes.

Users can also download (from the FOOTPRINT web site) databases of pesticide brands that have all the data required for FOOT-FS. The user can then import these pesticide brands into Pesticide Programme Builder (directly or using the Data Manager – see below).

2.3.3 My Equipment

In order to determine mitigation options it is necessary for the user to supply details of equipment used to apply the pesticides and what other equipment they might have available. The 'My Equipment' section allows the users to build up a list of sprayers and nozzles that they have available for applying pesticides. This list is then available when the user creates a risk assessment – the user simply selects the sprayer and nozzle (or sprayer/nozzle combination) for each product in the pesticide programme. Each sprayer and nozzle has a drift mitigation potential attached to it, which is then used in the assessment to calculate any drift reductions.

To aid this process further, the user can download (from the FOOTPRINT web site) and import data for a range of different commercial sprayers and nozzles, thus saving the user time and effort entering all the data themselves.

2.3.4 Data Manager

The Data Manager is a simple import/export tool that allows the user to manage and back up data that is stored in FOOT-FS. Data are held in central 'baseline' databases within the software. Over time the user could create a substantial amount of data in terms of farm and field details, pesticide brands and programmes and equipment. Hence, it is important that the user has a facility to make backups of this data so that they are not lost in the event that the user's PC fails. It also enables them to transfer data between PCs and (as described above) import standard data sets such as pesticide brands or equipment. The Data Manager allows the user to create FOOT-FS databases, and then they can copy data from their baseline databases into a FOOT-FS database. This FOOT-FS database can then be stored, moved and copied like any other file on a PC.

2.4 FOOT-FS Assessments

2.4.1 Introduction

The key function of the software is to provide the user with the ability to undertake risk assessments. This involves selecting a combination of a field scenario and a pesticide programme (and selecting equipment for that programme), then the selected data are used in the calculation routines.

The calculation routines undertaken are described in detail in Deliverable DL23 (Reichenberger et al., 2008b), in summary it includes the following processes:

- Calculations of Predicted Environmental Concentrations (PECs) and Time Weighted Average Concentrations (TWACs) for surface waters from spray drift, runoff and erosion including losses from sediments.
- Predicted leaching concentrations at the bottom of the soil profile
- The consideration of significant metabolites.
- Calculations of Toxicity : Exposure ratios (TERs) for fish, aquatic invertebrates, higher aquatic plants and algae. Both acute and chronic endpoints are considered where data exists in the Pesticide Properties Database (PPDB). Mesocosm studies are also included where these are reported in EU data dossiers for inclusion into Annex 1 of Council Direct 91/414/EEC.
- Conversion of TERs to FOOTPRINT 'Risk Scores' for simplifying interpretation.

The risk assessment outputs range from simple graphical approaches to detailed numerical outputs, presented in a way whereby the user can 'drill down' from the simple to the complex, depending on their personal requirements.

2.4.2 Creating assessments

There are essential two ways in which users can create and manage their FOOT-FS assessments

1. Quick Assessments
2. Saved Assessments

Quick assessments

The first approach is to simply select a farm/field and a pesticide programme and then run this combination through the calculation routines. The calculation routines will draw data directly from the baseline databases.

Saved assessments

The second approach involves selecting a farm/field and a pesticide programme and then saving this data into a new file. The user can either save a selection from the Quick Assessment facility or they can use a 'New Assessment Wizard' which will guide them through the process of selecting a combination that the wish to assess. Once saved, when the user runs the assessment the data will be drawn from the saved file and not the baseline databases.

The important aspect to note about this approach is when it comes to making amendments to the data, e.g. when exploring mitigation options, those amendments will be made only to the data in the saved file and not the users baseline databases. Thus maintaining the integrity of the baseline databases as building blocks for other assessments.

When a user has created and saved an assessment, they can open it again like any other file using the File-Open menu or using the Saved Assessments facility. They can then view the data in the assessment file by viewing the 'Summary of the current assessment'. Here they can also amend data in the file as required.

2.4.3 Assessment results / reporting and mitigation

Displaying assessment results

As described above, the approach to reporting the results is to initially provide a simple summary/overview of the assessment results. This is done graphically to highlight the key findings. The user can then drill down to detailed results should they require them. This approach ensures that the user is not immediately overwhelmed with a huge amount of data. It also helps direct them towards the key areas of concern (if there are any). Figure 15 provides an example of the summary screen that is initially presented.

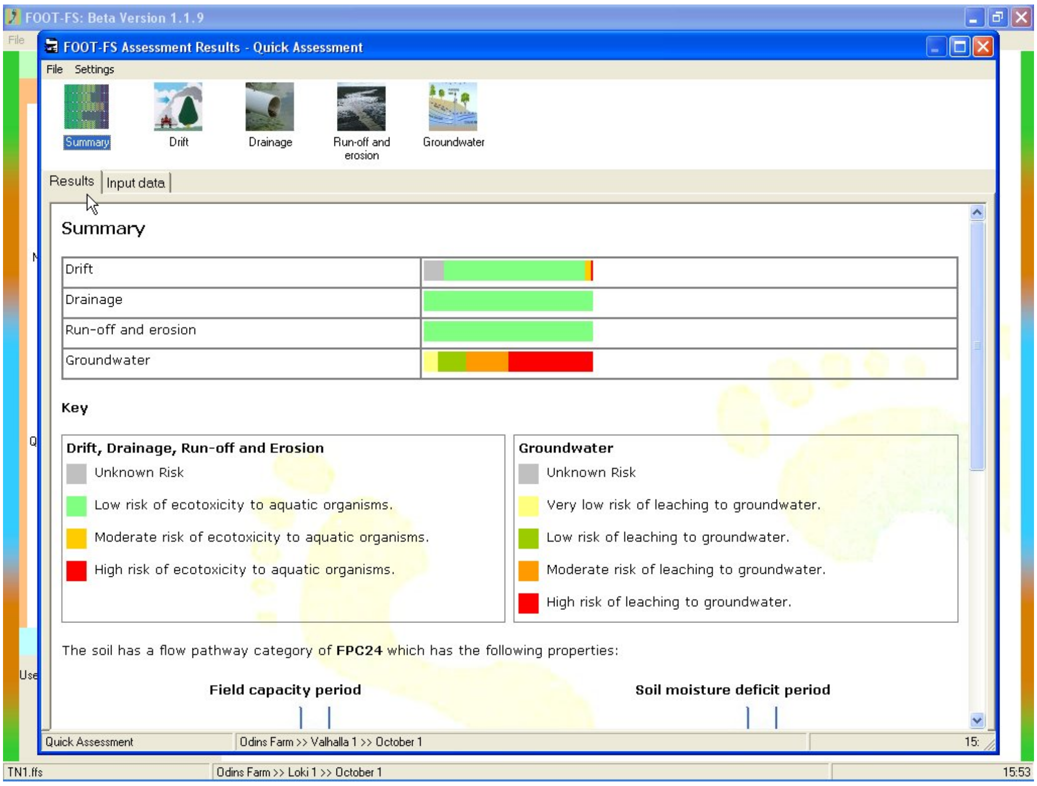


Figure 15 - FOOT-FS Assessment: Summary of results screen

Figure 15 shows the 4 pathways that have been assessed. Each has a colour-coded indicator bar next to it to represent any risks that have been identified (the colours used can be customised in the software settings). The indicator bar is comprised of the number of risk alerts relating to the seven different taxa from all active substances in the pesticide programme. The example in Figure 15 shows that in this instance there are some significant risks posed to groundwater and also a small risk from drift.

Having viewed the summary the user can then explore the results for different pathways in more detail. For example, Figure 16 shows the detailed results for drift.

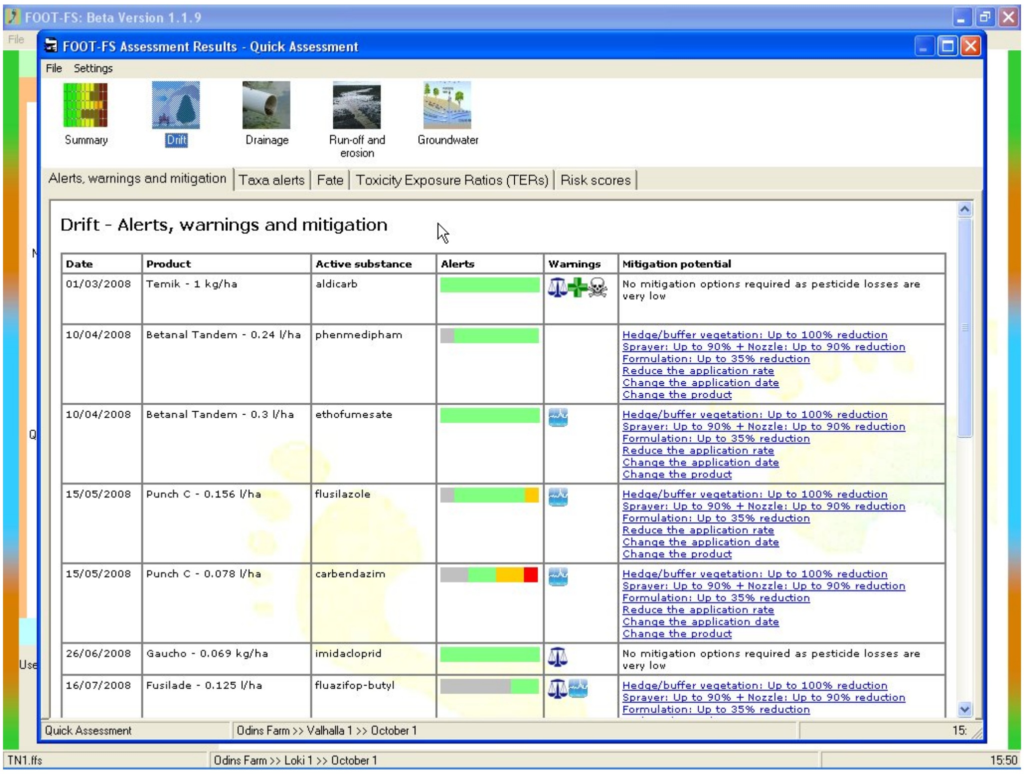


Figure 16 - FOOT-FS Assessment: Drift results screen

On the results screen for drift (shown in Figure 16) a similar risk indicator bar is used. This time it is used for individual pesticides within the pesticide programme. The example shown in Figure 16 has highlighted that there might be a risk from losses of carbendazim via drift.

Clicking on the Taxa alerts tab will show the risks that have been identified to specific taxa, using a simple icon system for alerts for different organisms. If the user wishes to see the results in numerical form, then clicking on the Fate tab will show the calculated losses and concentrations for different pesticides, clicking on the TER tab will display the Toxicity/Exposure Ratios (TERs) and the risk score tab will show the calculated risk scores. These three tabs are switched off by default upon installing the software, so the user has to specifically request in the software settings that these data are displayed.

Exploring mitigation options

On the screen shown in Figure 16, there is also a column called mitigation potential. Potential options to mitigate any risks are presented here. They are displayed as hyperlinks. If the user clicks on a hyperlink this opens the relevant data edit screen (previously access via 'My Data') and the user can implement some changes to mitigate any risks. Upon returning to the Results screen, the user is prompted to run the assessment again. Users can then see what impact the mitigation options they've implemented have on the risk assessment results.

Note: If the user is running a saved assessment then any changes/mitigation options implemented will be stored in the saved file. If the user is undertaking a quick assessment then these changes will be made to the baseline database.

2.5 The Toolbox

The toolbox contains a number of tools and facilities to compliment the FOOT-FS application. They include:

- A point source pollution audit
- Access to the PPDB
- A field screening tool
- Online best practice library
- Modelling results database manager and downloader
- Software update checker
- Software settings

2.5.1 Point source pollution audit

This tool provides a simple 'stand-alone' check-box questionnaire to assess the practices on the farm in relation to the potential risk of causing point source pollution from pesticides. It covers general practices, the pesticide store, preparation and waste management. The user simply 'ticks' the boxes that apply to their practices. Each question also has links to additional information, specific to the question including best practice definitions, and photographs (provided by the European project TOPPS) of poor and good practices. When complete, a report is displayed highlighting where improvements could be made and the likely cost and effectiveness of implementing the suggested practices. The photographs of good and poor practices are also available from links within the report.

2.5.2 Access to the PPDB

The FOOTPRINT Pesticide Properties Database (PPBD) is described in detail in Deliverable DL24 (Lewis et al., 2007). The facility in the toolbox provides direct access to the PPDB from the FOOT-FS Shell. The user can choose to either access the online version of the database - which is then displayed in a web browser - or they can view the database that is installed locally on their PC as part of the FOOT-FS software. Viewing the local database will display only the pesticide data that is used within the risk assessment modelling. Viewing the online database will display the most up-to-date data for the pesticide as it is updated on a daily basis. Access to the local database is provided using a simple interface. Down the left side of the interface is an 'A to Z' of all the pesticides in the database, clicking on an item in the list will show the data for that pesticide on the right. The user can also search for a pesticide by entering a search term in the top left and clicking on the search button.

The PPDB stored within FOOT-FS can be updated with new versions. This is described in the section on Settings below.

2.5.3 Field screening tool

Any specific farm may have tens or even hundreds of fields, so to undertake a full FOOT-FS risk assessment of all the fields would be time consuming. Thus ideally a full risk assessment should only be undertaken on those fields of most concern. To help the user select the fields of most concern, a simple field screening tool has been developed that can be used prior to undertaking a full risk assessment. This simple tool looks at a number of risk factors to determine the likely susceptibility of a field to exporting pesticides to surface water via drift, drainage, surface runoff and erosion or to groundwater via leaching. These factors include: distance to a water body, proneness to soil capping, slope, presence of a shallow or karstic substrate, presence of wells, boreholes and drainage networks, permeability of the soil, proneness of soil to waterlogging and the type of sprayer used. If the screening identifies any potential susceptibility for exporting pesticides surface water or groundwater then it is suggested that a full FOOT-FS risk assessment be undertaken.

2.5.4 Online best practice library

The purpose of this tool is to provide a repository of some of the key best practice documents and online resources relating to the pesticide use best practice. As this type of material is likely to vary between different EU member states, a separate page will be created for each language, and thus specific documents for that country will be available on that page. Additionally, as they are stored online it will be a straightforward process to update any document with new versions, as they are not stored/installed with the FOOT-FS software.

2.5.5 Modelling results database manager and downloader

The calculations of pesticide losses via run-off and erosion, drainage and leaching are made in FOOT-FS by retrieving data from a set of databases known as modelling results databases. These contain results for a range of conditions across the whole of Europe. As such the amount of data they contain is large – approximately 70-100 Gigabytes of data. This amount of data cannot be installed as part of a standard FOOT-FS installation and most users will only need a small fraction of these data. To overcome this problem a modelling results database download tool has been developed. Crop type, climate zone and percentile are used divide the results databases into approximately 8000-9000 files and these are stored on the FOOTPRINT project web server.

This tool has a number of different functions. Firstly, it displays what data the user has already installed. Secondly, the user can see what data are available to download. The tool contacts the web server and then displays which data are available. The user can then select which data they want to download simply by ticking the relevant boxes and then clicking on the download button. The software then automatically downloads and unzips the data. The user does not have to manage the data themselves other than choose a folder to save the data in.

If the user attempts to undertake a FOOT-FS risk assessment with out downloading the appropriate modelling results databases, the software will prompt the user to download them. The software will then automatically select the required databases and then download and install them as described above.

2.5.6 Software update checker

A key part of any modern software system is to be able to update the software. Part of this process is for the user to be notified when updates are available. When the user activates this facility it contacts a web server to obtain information on the latest version that is available. If a new version is available the user is informed and directed towards the web site where they can download the update.

2.5.7 Software settings

The software settings section of FOOT-FS provides a number of facilities to allow the user to customise their version of FOOT-FS to their requirements. This includes:

- General settings to determine what dialog screens to display when the software starts

- What version of the PPDB to display – local or internet
- Whether to have icons or text as warnings in the results display
- What colours to use for the different risk categories in the risk indicator bar
- Whether to display the pesticide property data prior to running an assessment, and thus allow the user to amend the property values
- Options to display fate, TER and risk score data in the assessment results
- The style of the risk indicator bar, i.e. is it variable length depending the number of pesticides used or a fixed length.
- The default percentile to use for run-off and erosion and drainage results data
- Default values to be used when calculating concentrations of pesticides in surface water, including bulk density of sediment, depth of the upper sediment layer, depth of the lower sediment layer, organic carbon content of sediment and porosity of sediment.

The settings also contain a facility to automatically download and install new versions of the FOOTPRINT PPDB. As described previously the FOOTPRINT PPDB is updated on an almost daily basis, e.g. with new active substances or new data for existing substances. So in order to ensure that FOOT-FS users have the most up to date pesticide properties data, a facility is required to update the FOOTPRINT PPDB within FOOT-FS. In the settings the user can check for updates to the FOOTPRINT PPDB to see if they have the latest version. If they do not have the latest version they can either automatically download/install the new version or if they have manually downloaded the file they can also install that file using the facility in the settings.

2.6 FOOT-FS Validation

A comprehensive report of all the testing, piloting and evaluation exercises undertaken for FOOT-FS is available in Deliverable DL37, so only a summary is presented here. Validation activities have included:

- Ensuring that the outputs from the FOOT-FS software are comparable with those that would be provided by the original models, taking in to account the intermediary modelling stage and the broad-based spatial descriptions of climate and soil that would invariably introduce some deviation from the parent models.
- Ensuring that FOOT-FS meets its design objectives and is able to raise user awareness regarding agricultural pesticide use and the aquatic environment particularly with respect to on-farm planning and mitigation options.

- Ensuring that it meets the needs of end-users, is user-friendly, free (as far is reasonably possible) of bugs and is operational on a range of commonly used computers and operating systems.

This has been achieved by undertaking a number of in-house testing activities, organising a number of workshops in a range of EU Member States and holding a information relay workshop in conjunction with the FOOTPRINT Final Conference at Giessen University in Germany.

The findings from the various evaluation activities have all been used to correct, polish and improve the beta-version of the FOOT-FS software (as described in Deliverable DL26 (Lewis & Tzilivakis, 2007)) and led to the final version (as described in Deliverable DL34 (Lewis & Tzilivakis, 2009a)). Separate reports have been produced that provide greater detail than herein for the piloting workshops (Deliverable DL31 (Lewis & Tzilivakis, 2008)) and the FOOT-FS information relay workshop (Deliverable DL40 (Lewis & Tzilivakis, 2009b)).

3 THE SPATIAL TOOLS FOOT-CRS AND -NES

The two spatial tools FOOT-CRS and FOOT-NES have many similarities and common features:

- They belong to the same software development project.
- They are installed with the same installation package (FOOTPRINT.msi).
- They share several .dlls
- They have the same modular structure.
- The respective modules in FOOT-CRS and FOOT-NES are similar in their appearance and functionality.
- The two tools have almost the same system requirements.

However, there are many subtle, but important differences between FOOT-CRS and FOOT-NES. For this reason, the two tools are described separately in the two following sections 3.1 and 3.2.

To avoid repetition, the modular structure common to both FOOT-CRS and FOOT-NES is presented in the following. FOOT-CRS and FOOT-NES have been programmed as add-ons (more precisely, toolbars; Fig. 17) in the ESRI ArcGIS software. The tools consist of 5 modules (Fig. 18):

- Data Manager
- Pesticide Scenario Manager

- Dominant Pathways Module
- Modelling Module
- Communication and Reporting Module

Figure 17 - The FOOT-CRS and FOOT-NES toolbars (state: 20 January 2010)

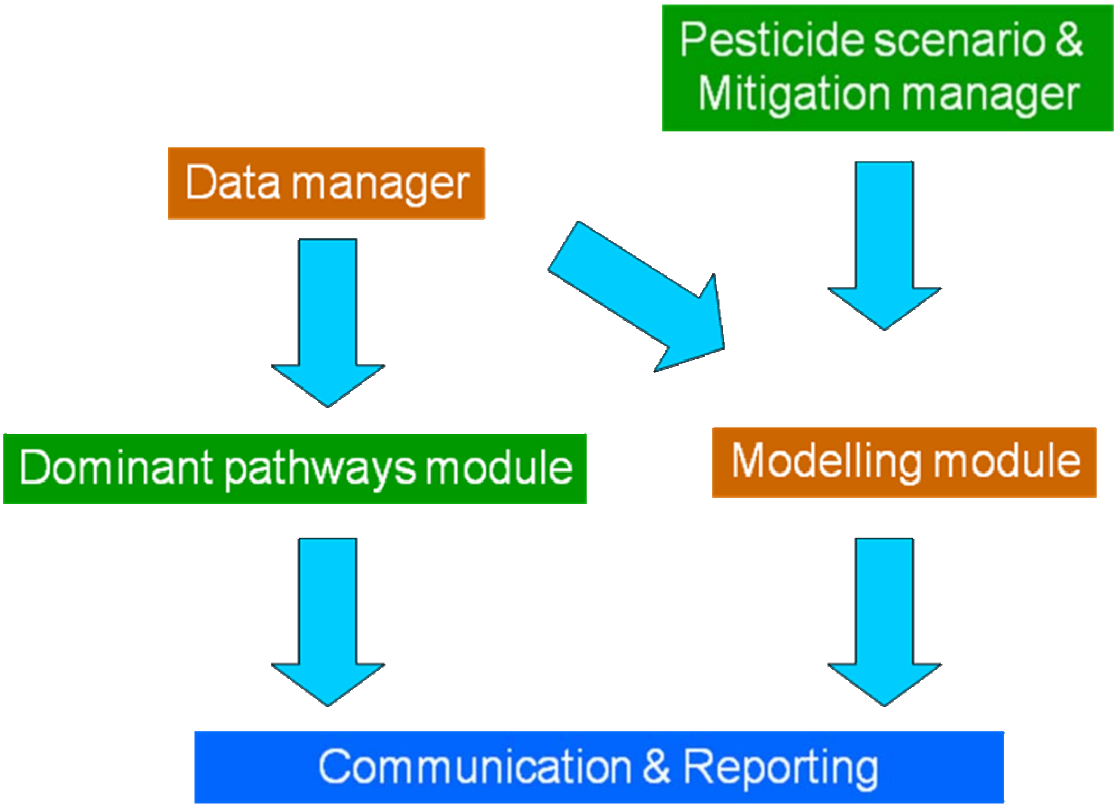


Figure 18 - Logical structure and data flow in FOOT-CRS and FOOT-NES.

The general purpose of the Data Manager is to administrate the input data for the Modelling Module (apart from the pesticide application scenarios) and for the Dominant Pathways Module. Moreover, it facilitates the import of the user's own data, in case the user wants to replace one or more of the FOOTPRINT default data sets (soil, land cover, land use, etc.) with own datasets.

In the Pesticide Scenario Manager, the user specifies the pesticide application(s) to be simulated. The module also allows to explore the effects of mitigation (= risk reduction) measures.

The Dominant Pathways Module produces maps of the relative importance of the different soil-related contamination pathways (surface runoff, erosion, drainage, leaching), and also a map giving the dominant contamination pathway for each polygon.

The Modelling Module does the actual pesticide-related calculations in FOOT-CRS and FOOT-NES. It

- reads and processes the input from the Pesticide Scenario Manager
- accesses the currently active agro-environmental scenario database
- extracts values from the various Modelling Databases
- calculates leaching concentrations, pesticide losses from fields, pesticide inputs into the surface water network, concentrations in surface water at the catchment outlet (FOOT-CRS) or concentrations in surface water and sediment (FOOT-NES) in hypothetical edge-of-field water bodies.
- produces maps and spatial and temporal CDFs (tables and graphs).

The tasks of the Communication and Reporting Module are to display the output variables produced by the Modelling Module (maps, spatial and temporal CDFs) and the maps produced by the Dominant Pathways Module.

3.1 FOOT-CRS

3.1.1 Overview of FOOT-CRS (Catchment and Regional Scale)

FOOT-CRS is a GIS-based tool for pesticide risk assessment at the catchment scale. It is to be used at the catchment level by ‘water quality’ managers, i.e. regional/local authorities, water agencies and water companies. The emphasis in FOOT-CRS is on i) identifying the areas most contributing to the contamination of water resources by pesticides, and ii) defining and/or optimising action plans at the scale of the catchment.

In contrast to the national-scale tool FOOT-NES, FOOT-CRS uses the real surface water network, and Predicted Environmental Concentrations in surface water (PECsw) are calculated at the catchment outlet (i.e. for one point in space).

For the calculation of pesticide inputs into surface water via surface runoff and erosion, a routing to the surface water network is performed on a grid basis and the load reduction by reinfiltration or redeposition is explicitly calculated. Drift input calculation is done on a vector basis, considering mitigating landscape elements like hedges and riparian vegetation.

Finally, FOOT-CRS produces temporal CDFs of Predicted Environmental Concentrations in surface water (PECsw) at the catchment outlet (i.e. for one point in space), for different pesticide input pathways. These CDFs can e.g. be used to determine the return period of a given monthly maximum concentration for the pesticide of concern.

In total, the FOOT-CRS modelling module produces the following output for surface water:

- Maps and spatial cumulative distribution functions (CDFs) of
  - pesticide losses from fields and
  - pesticide inputs into the surface water network
- Temporal CDFs of Predicted Environmental Concentrations in surface water (PECsw) at the catchment outlet. From these, exceedance frequencies and return periods of given monthly maximum concentrations can be directly calculated.

3.1.2 System requirements

To install and run FOOT-CRS, the user's system must meet the following requirements:

- OS: Windows XP or Vista (the tool has been developed on XP, but also been tested on Vista)
- Installed software:
  - ArcGIS 9.3
  - ArcGIS Spatial Analyst extension
  - ArcGIS .NET Support
  - Microsoft .NET Framework 2.0 or higher
  - Microsoft Access 2003 or 2007
- User account: The user needs admin rights for installation, but not for running the tool

3.1.3 FOOT-CRS requirements

All existing modules of FOOT-CRS have been developed in the programming language C# ("C sharp") by Björn Feisel (iNovaGIS), except for the FOOT-CRS Pesticide Scenario Manager module, which has been programmed in VB.NET by Moritz Wurm (iNovaGIS). The FOOT-CRS Pesticide Scenario Manager has been adapted from the FOOT-NES Pesticide Scenario Manager, which was originally programmed by David Windhorst (UG) in VB.NET and then extended by the selection and handling of mitigation measures by Moritz Wurm (iNovaGIS). The Pesticide Scenario Manager, FOOT-NES and FOOT-CRS have now been integrated in a single installation package (.msi), and that the Pesticide Scenario Manager is now part of the FOOT-NES and FOOT-CRS toolbars.

3.1.4 The FOOT-CRS Data Manager

The general purpose of the Data Manager is to administrate the input data for the Modelling Module (apart from the pesticide application scenarios) and for the Dominant Pathways Module (cf. Fig. 18). Moreover, it facilitates the import of the user's own data, in case the user wants to replace one or more of the FOOTPRINT default data sets (soil, land cover, land use, etc.) with own datasets. As a consequence of importing one or more user datasets, a new agro-environmental shapefile and database have to be created by the Data Manager.

The FOOT-CRS Data Manager is organized in 7 tabs:

- Project
- General
- Land Cover / Land Use Map
- Soil map
- Landscape / Mitigation features
- Surface water network
- Discharge

The currently active settings on all tabs of the Data Manager can be saved as a project. The projects are necessary because the Modelling Module and the Dominant Pathways Module need to know what input data (incl. agroenv. scenario DB and shape) they shall use. That means, when running a pesticide application scenario in the Modelling Module (cf. section 3.1.8 of chapter 4), the user must make sure that the AOI (area of interest) shapefile used by the Pesticide Scenario Manager (cf. section 3.1.5 of this chapter) to create the pesticide application scenario matches with the agroenv. scenario database that is currently active in the Data Manager → The right project must be loaded in the Data Manager before starting a run with the Modelling Module.

The FOOT-CRS Data Manager is very similar to its counterpart in FOOT-NES. In fact, both Data Managers are the same piece of software (i.e., they share the same .dll), but dynamically adapt their features to the tool in which they are used.

Tab Project

This tab (Fig.19) is the same as in FOOT-NES, except that apart from the agro-environmental scenario map and database, also a landscape feature / land cover map is generated. Here the user can create and administrate projects, and create files required for running a FOOT-CRS assessment. If the user saves a project and clicks on "create" on the project tab, the data manager will create:

- a user-defined agro-environmental scenario shapefile (single-part) and database (subsequently, the names and paths of the new shapefile and database will appear on the General Tab as currently active agro-environmental scenario shape and database).
- a user-defined landscape feature / land cover map (this map will be used by the Modelling Module in the surface runoff routing and in the drift calculation procedure). There are four options for the user here, determining whether a landscape feature shapefile, a mitigation feature shapefile, both or none of them shall be included in the procedure that creates the landscape feature / land cover map.

To be able to create an agro-environmental . scenario map and database, the user must have specified the following input data:

- Climate map
- Land cover / land use map (+ assignment performed)
- Soil map and soil table (+ assignment performed)
- discharge
- catchment boundary shape (on the surface water network tab)

It has to be noted that, in contrast to FOOT-NES, it is essential for the meaningfulness of the FOOT-CRS surface water modelling output that the agro-environmental scenario shape does not contain holes (i.e. it must cover the whole catchment area). Consequently, these input files must not contain holes either.

To be able to create a landscape feature / land cover shapefile, the user must have specified the following input data:

- Land cover / land use map (+ assignment performed)

Specifying a landscape feature shapefile and/or mitigation feature shapefile (with assignment performed) is only optional.

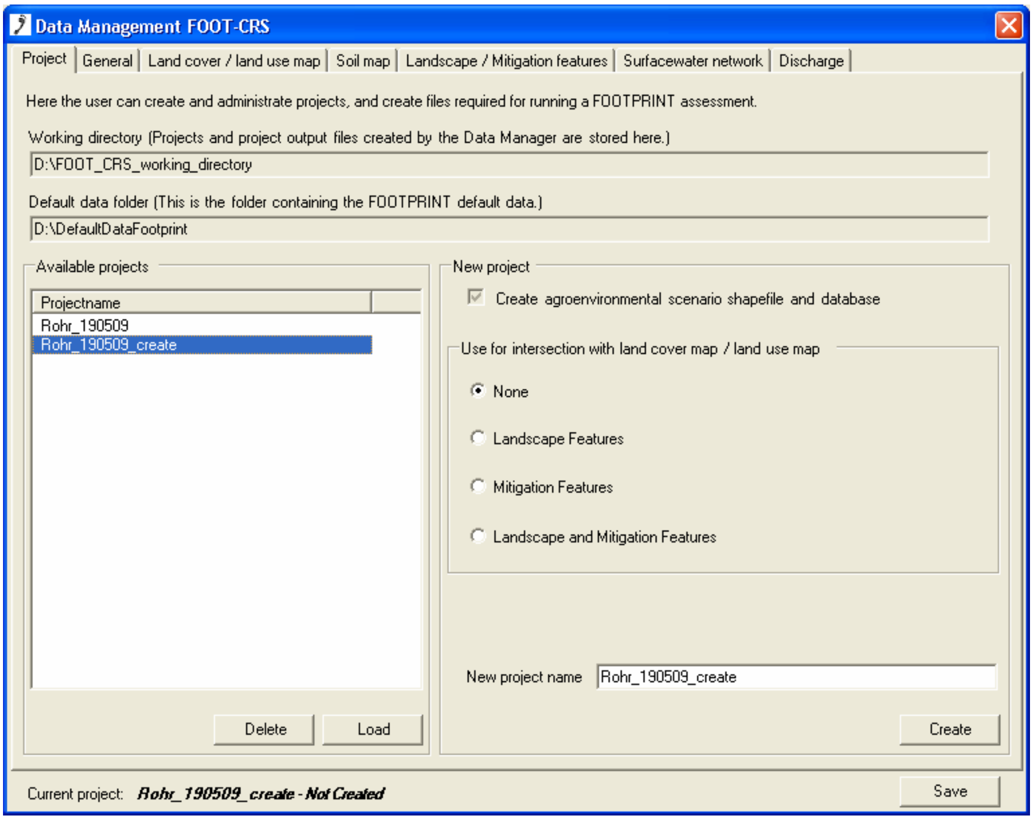


Figure 19 - The FOOT-CRS Data Manager, Tab "Project"

Tab General

This tab (Fig. 20) is the same as in the FOOT-NES Data Manager (cf. section 3.2.4), except that additionally a Digital Elevation Model (DEM) is required and also three optional groundwater-related data sets can be specified.

In the "General" tab, the names and paths of various data sets required for creating projects or running an assessment are specified:

- *Default data folder:* This is the folder where the FOOTPRINT default data are stored (this path will become relevant when the final version of FOOT-CRS is distributed along with European-level default data sets)
- *Working Directory:* This the folder where the Data Manager stores the files and projects it creates.
- *Agroenvironmental scenario shapefile:* This is the currently active agro-environmental scenario shape, i.e. the one currently to be used by the Dominant Pathways module. It can be either the default or an user-defined agro-environmental scenario shape (depends on the project).

  Note: The modelling does not work with this shape, but with the AOI shape specified in the Pesticide Scenario Manager, which is either an agro-environmental scenario shape or a subset of one.

- *Agroenvironmental scenario database:* This is the currently active agro-environmental scenario database, i.e. the one currently to be used by the Modelling module and the Dominant Pathways module. It can be either the default or an user-defined agro-environmental scenario DB (depends on the project). Note that the active agro-environmental scenario shape and database must match each other.
- *Control modelling database:* This is an Access database which lists the names of the various Modelling databases with MACRO and PRZM results. In more detail, for each crop/climate combination it gives the name of the corresponding gw database, and for each crop/climate/appmonth combination it gives the name of the corresponding sw database. The control modelling database has to be in the same folder as the Modelling databases.
- *FOOTPRINT climate zones shapefile:* This is the shapefile containing the FOOTPRINT climate zones. It cannot be edited or replaced by the user.
- *SUGAR map:* Map of the FOOTPRINT SUGAR (Surface Water / Groundwater Contribution) Index. This can be the European level default SUGAR map or a more detailed map based on the user's own data.
- *FOOTPRINT classification database:* This database contains the tables to fill the assignment boxes on the Land Cover / Land Use tab, the soil tab and the landscape / mitigation tab.
- *Digital Elevation Model:* This is the DEM to be used in the routing procedure of surface runoff and eroded sediment.
- *Unsaturated zone thickness / Aquifer properties / Flow concentration*: These are optional datasets which can be displayed along with the PECgw/SUGAR map to aid in groundwater risk assessment. However, they are not used for any calculations.

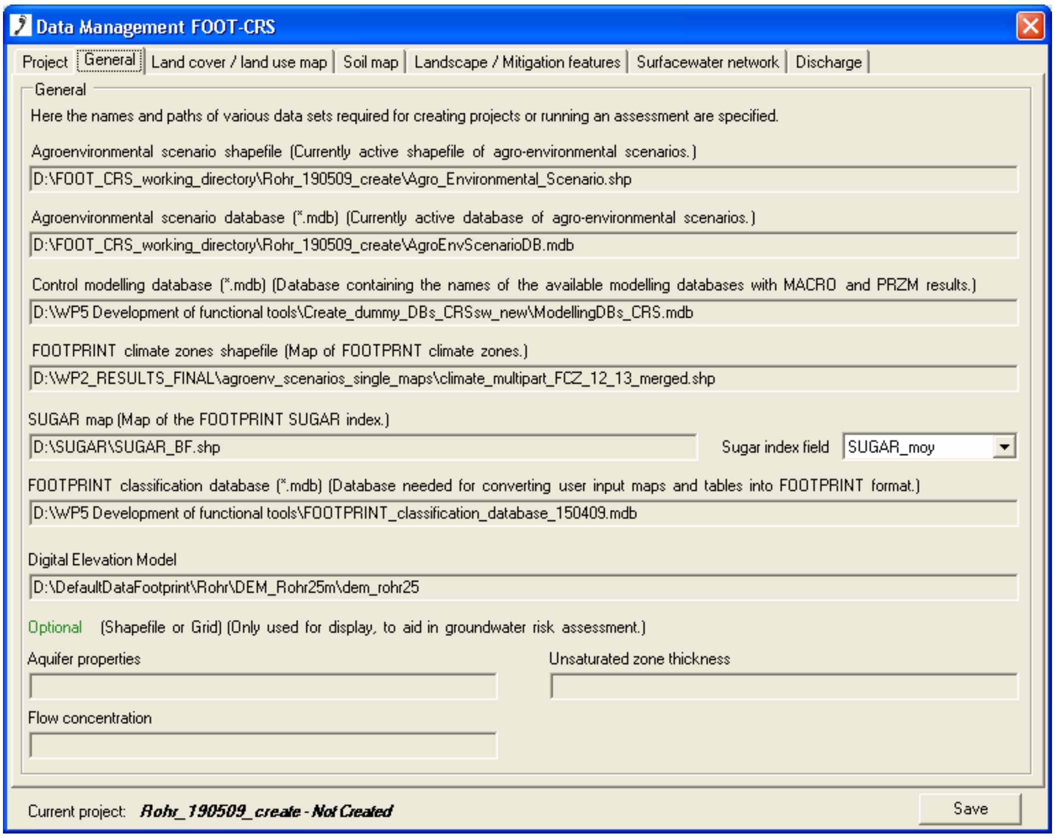


Figure 20 -The FOOT-CRS Data Manager, Tab "General"

The Land Cover / Land Use Tab

This tab (Fig. 21) is identical to the one in FOOT-NES, with one exception: While in FOOT-NES the user needs to specify two administrative levels, in FOOT-CRS it is only one administrative level. This level will be available as aggregation options for pesticide losses from fields, inputs into surface water bodies and PECgw to spatial CDFs in the FOOT-CRS Modelling Module. In the Land Cover / Land Use tab, the user can import own land cover and/or land use data in shapefile format (or just specify the default land cover / land use map). The Land Cover / Land Use map must contain both land cover (type of cover of the soil) and land use (area fractions of crop groups based on agricultural statistics). Consequently, the shapefile the user specifies must contain the following columns (fields) in its attribute table:

- Administrative code field on which the agricultural statistics are based (this administrative level is then available as an aggregation option for pesticide losses and inputs to CDFs in the Modelling Module). It has to be specified in the listbox "administrative code field".

- The column that contains the land cover classes (e.g. CLC classes). It has to be specified in the listbox "Land Cover Code field".

- Various columns containing the area fractions of the various crop groups in the polygons of the shapefile (Note that the LC/LU map can be a multi-part or a single-part shapefile; the Data Manager doesn't mind either format. But the user must decide before creating his/her LC/LU shapefile which format is more appropriate for his/her purpose!)

In the group box "Land Cover", the user can assign FOOTPRINT land cover codes (CORINE Land Cover format) (e.g. 211 = "non-irrigated arable land") to the land cover codes of his/her own map LC/LU map. If the user's land cover codes are already in CLC format (as is the case for the default LC/LU map), an automatic assignment can be performed by clicking on the text "automatic assignment".

In the group box "Land Use", the user can assign FATE crop groups or land use classes (e.g. VALUE_72 = barley) to the land use classes of his/her own LC/LU map. If the user's land cover codes are already in FATE format (as is the case for the default LC/LU map), an automatic assignment can be performed by clicking on the text "automatic assignment".

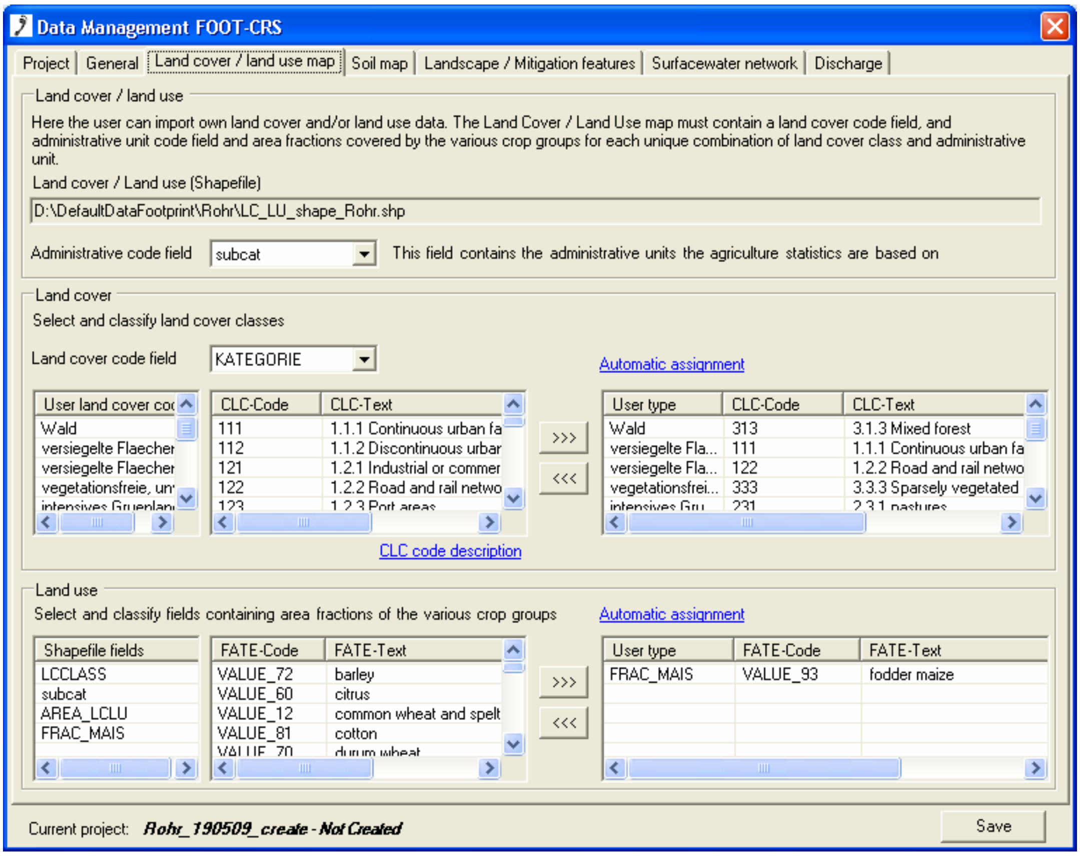


Figure 21 - The FOOT-CRS Data Manager, Tab "Land Cover / Land Use map"

Tab Soil map

This tab (Fig. 22) is identical to its counterpart in FOOT-NES. In the tab “Soil map”, it the user can import own soil data (or just specify the default soil map and table). The user has to specify both a soil map (shapefile) AND a soil table (.dbf).

The map (shapefile) must contain a column with the soil mapping units (SMU).

The soil table (.dbf) must contain these columns:

- Soil Mapping Unit (SMU) (which must have the same SMU codes as the SMU column in the soil shapefile)
- Soil Typological Unit (STU)
- The area fraction covered by each STU occurring in an SMU.

Note: Usually an SMU contains more than one STU. If, however, there is only one STU per SMU (might occur in detailed user soil maps), the area fraction covered by this STU is 1. However, even is there is only one STU per SMU, the soil table must be physically different from the attribute table of the soil shapefile.

In the lower part of the tab the user can assign FOOTPRINT soil types (FST) and Flow Pathway Categories (FPC) to his/her own STUs, both manually and automatically.

Since in the case of manual assignment the user will usually not know the FST corresponding to his/her STU beforehand, a link will be placed on the tab that opens the FOOTPRINT soil selector software by John Tzilivakis (UH).

Analogously to the land cover / land use tab, there is also an automatic assignment in place, for the case that the user’s soil types are already in FST format. To enable an automatic assignment, the user must specify an FST column and an FPC column in his/her soil table. To increase the performance (calculation speed) of the automatic assignment procedure, it is possible that the file format of the soil table will be changed from .dbf to .mdb before the release of FOOT-CRS to the public.

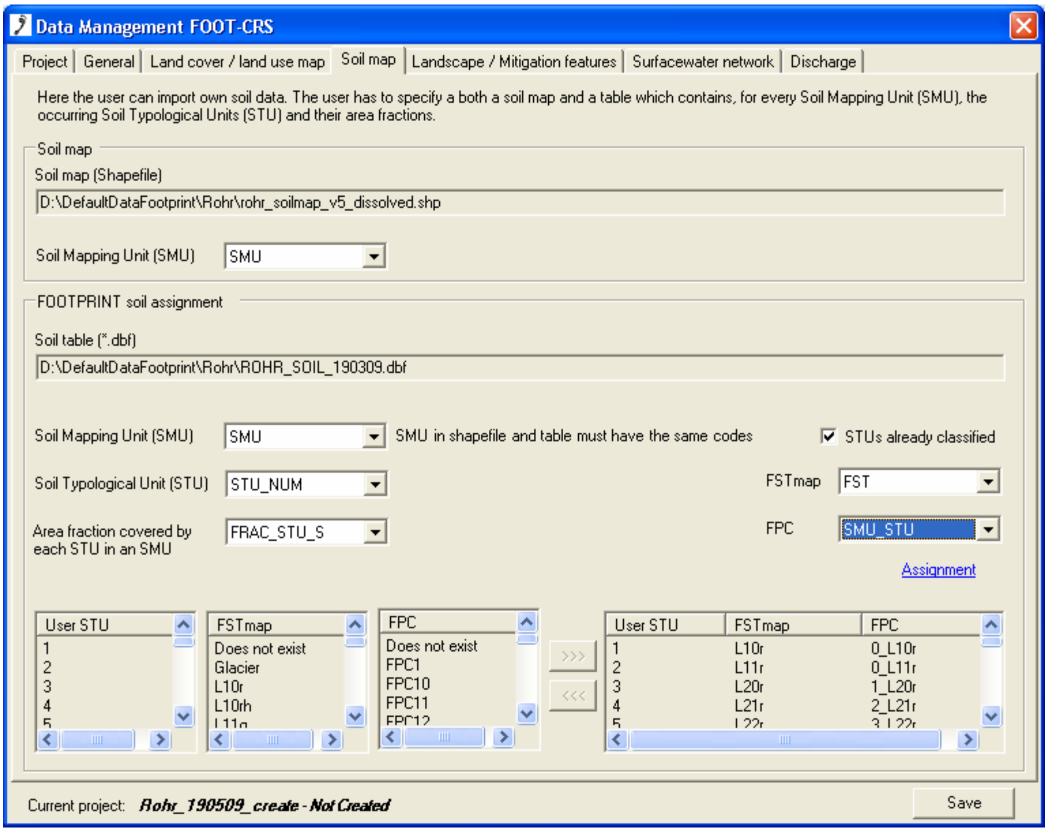


Figure 22 - The FOOT-CRS Data Manager, Tab "Soil map"

Tab Landscape / Mitigation features

In this tab (Fig. 23), the user can convert existing maps (shapefiles) containing landscape elements that reduce pesticide inputs into surface waters, like hedges, grassed buffers or forests, into FOOTPRINT format. The only difference between landscape feature map and mitigation feature map is that the former is meant to contain real (i.e. observed) landscape elements and the latter hypothetical (i.e. user-drawn) ones.

The landscape feature / mitigation feature map (shapefile) must contain a column containing the user's landscape feature classes. It has to be selected in the listbox "landscape field".

In FOOT-CRS, the user can draw a landscape feature / mitigation feature shape oneself with the Landscape Feature Digitizer (part of the FOOT-CRS toolbar), making use of the Editor functionality in ArcGIS (cf. section 3.1.6).

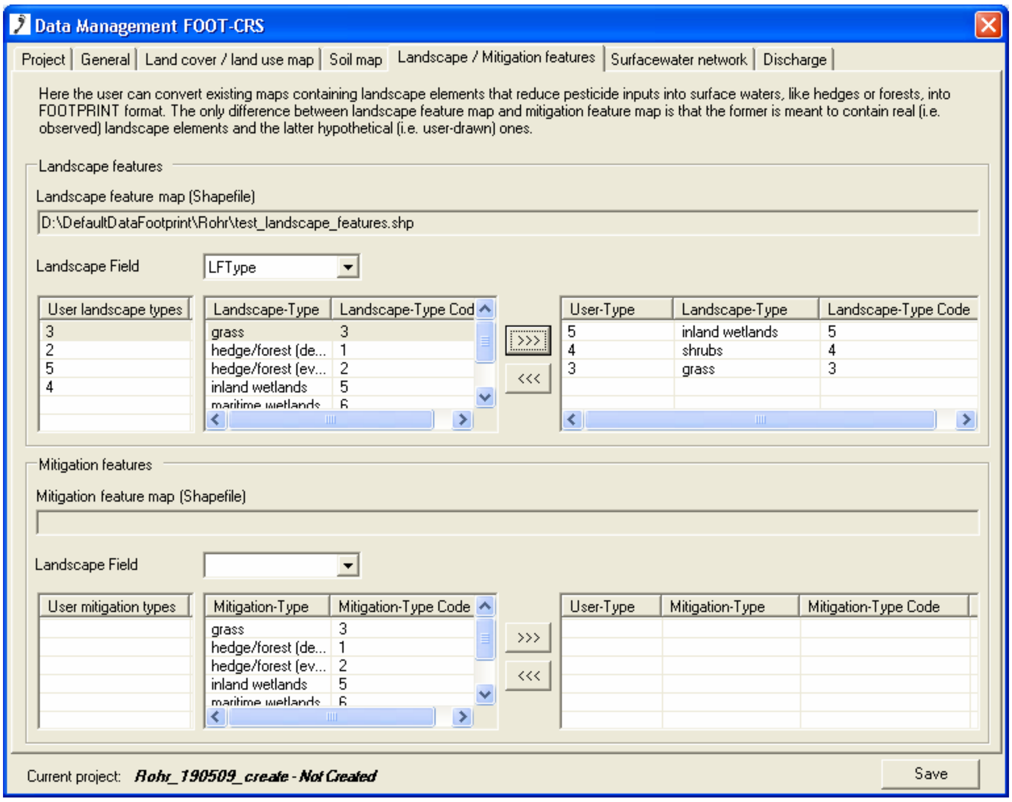


Figure 23 - The FOOT-CRS Data Manager, Tab "Landscape / Mitigation features"

Tab Surface water network

This tab (Fig. 24) is completely different from the tab "Surface water body characteristics" in FOOT-NES. The reason is that while FOOT-NES uses hypothetical edge-of-field surface water bodies, FOOT-CRS uses an observed surface water network.

In this tab, the user can specify a surface water network map in shapefile format (or just specify the default surface water network map from the CCM 2.1 dataset (Vogt et al., 2007a; Vogt et al., 2007b)).

If not all attributes required to run an assessment are available as columns of the network map shapefile, values of river width and depth for each calendar month can be estimated internally according to the methodology of Pistocchi and Pennington (2006) from river discharge for each calendar month (routines have been formulated, but not been implemented yet), and default sediment parameters (OC content, depth, bulk density) according to FOCUS (2001) can be used.

On this tab the user also has to specify a catchment boundary shape, defining the catchment of interest.

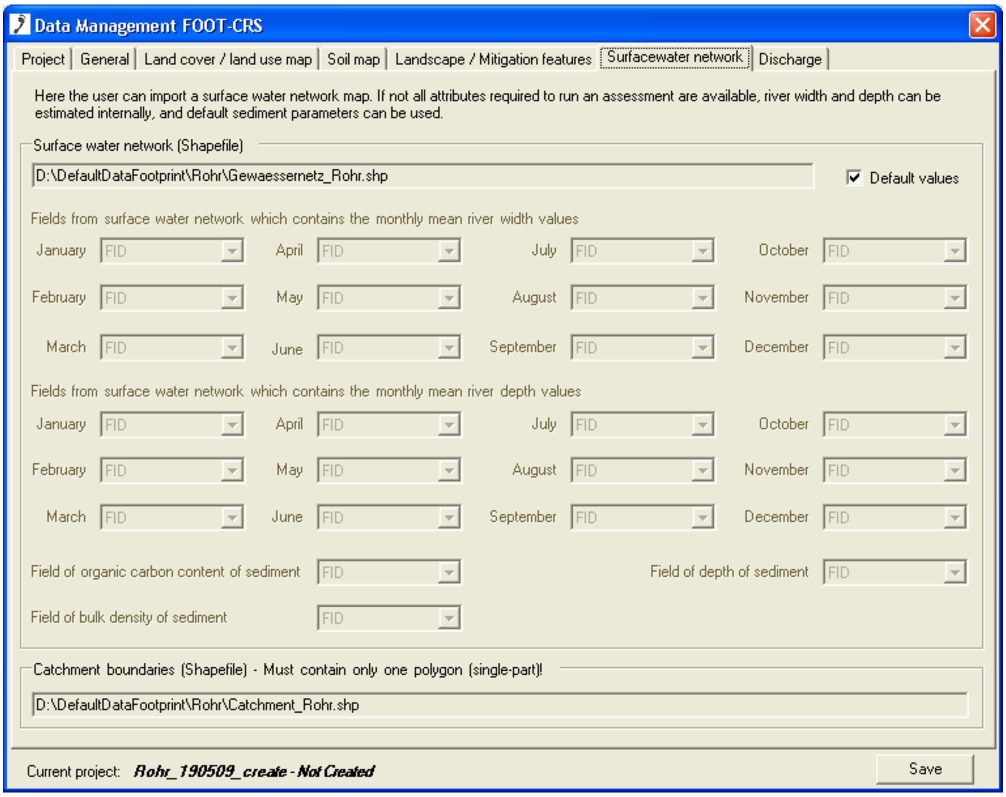


Figure 24 - The FOOT-CRS Data Manager, Tab "Surface water network"

Tab Discharge

The tab (Fig. 25) is identical to the discharge tab in FOOT-NES (cf.section 3.2.4). Since the FOOT-CRS user needs to have the ArcGIS Spatial Analyst extension installed anyway for the drift calculations and the surface runoff routing, the FOOT-CRS user can always specify the discharge in grid format here. The discharge grids are later processed using the zonal statistics function, for which the Spatial Analyst is needed.
However, also the vector-based methodology for discharge processing developed for FOOT-NES will be available as additional option in the final version of FOOT-CRS.

In the discharge tab, the user has to specify maps of mean discharge for each calendar month (or just specify the default discharge maps (UNH Composite Runoff Fields; Fekete et al., 2000)). Note that not maps of actual river discharge (in e.g. m^3 d^{-1}) are required, but maps of area-specific discharge, i.e. excess water from a unit area that runs off to rivers (mm d^{-1}), e.g. calculated from a climatic water balance.

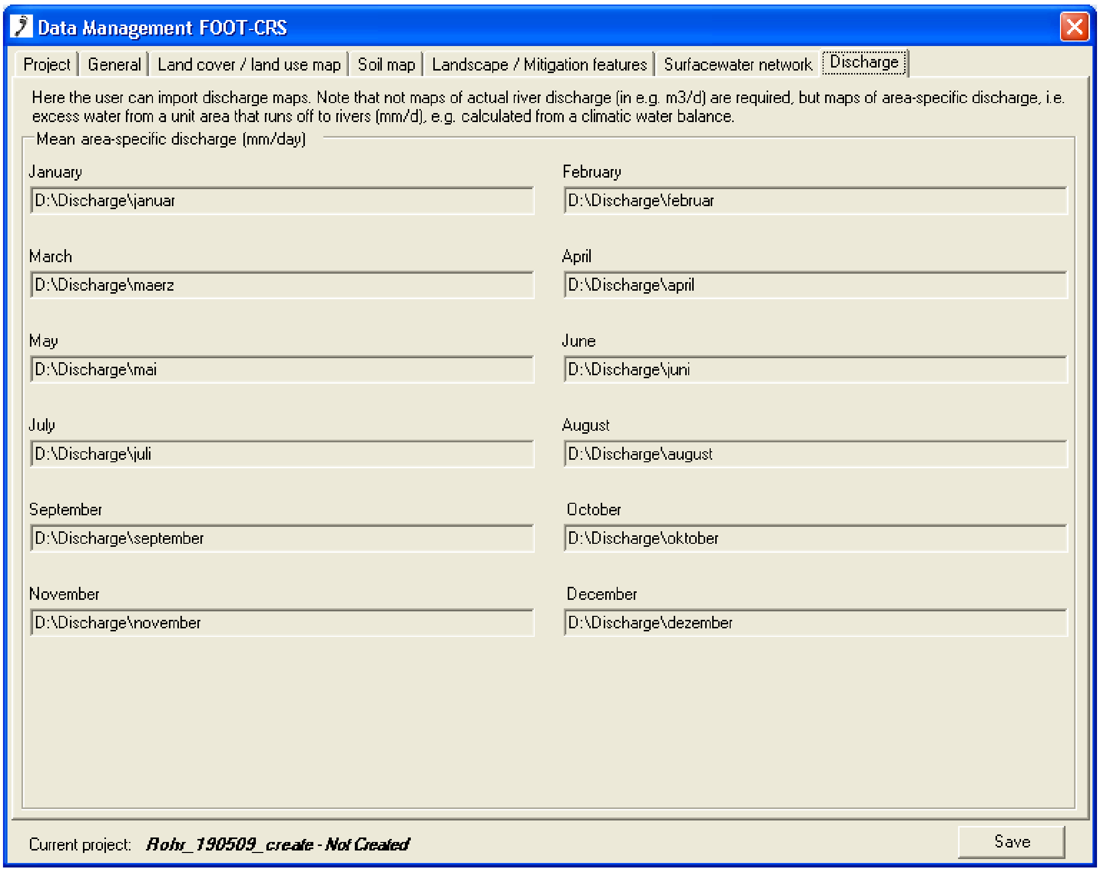


Figure 25 - The FOOT-CRS Data Manager, Tab "Discharge"

3.1.5 The FOOT-CRS Pesticide Scenario Manager

In this module, the user specifies the pesticide application(s) to be simulated. The module also allows to explore the effects of mitigation (= risk reduction) measures related to drift reducing technology.

The FOOT-CRS Pesticide Scenario Manager has recently become available. It has been adapted from the FOOT-NES Pesticide Scenario Manager (cf. section 3.2.5). The most important adaptations were:

1. Tab "Pesticide": removal of the box containing the percentiles for drainage, runoff and erosion
2. structure of the .fps file: no writing of records with different drainage/runoff/erosion percentiles into the fps file (this is coupled to 1.)
3. Tab "Spatially variable mitigation measures": removal of this tab (these mitigation measures are input by the user in a georeferenced manner through the landscape feature and/or mitigation feature shapefile).

4. structure of the .fps file: Also for untreated polygons records must be written to the .fps file. The reason is that for all polygons in the catchment, precipitation values must be extracted from the modelling databases. Hence, for the untreated polygons “dummy applications” (with application rate = 0, percentage treated = 0, and application month = median of application months in the treated polygons) are written to the .fps.

Since the changes necessary to adjust the Pesticide Scenario Manager to FOOT-CRS requirements were moderate, we opted for a dynamic adaptation, analogously to the Data Manager. That is, the FOOT-NES and FOOT-CRS Pesticide Scenario Managers are the same piece of software, but dynamically adapt their features to the tool in which they are used.

Setting up the Pesticide Scenario Manager

When opening the Pesticide Scenario Manager the first time, the user is prompted to make some settings in the Setup window (Fig. 26):

- Specify the path and filename of the version of the Pesticide Properties Database (PPDB; Lewis et al., 2007) to be used.

Specify the path and filename of the agro-environmental scenario database to be used. In fact, the Pesticide Scenario manager uses only one table in the agro-environmental scenario database, and this table is also the same in all agro-environmental databases. For convenience of the user, the selection under “select table” jumps automatically to this table (“FCR_vs_EUROSTAT_vs_FATE_text_num”). However, the selections of the right columns in this table have to be done manually exactly according to Fig. 26. The table “FCR_vs_EUROSTAT_vs_FATE_text_num” contains the relations between the 42 FOOTPRINT crops (which are being modelled) and the FATE crop groups (for which there are area fractions contained in the agro-environmental scenario database), and the available application types for each FOOTPRINT crop.

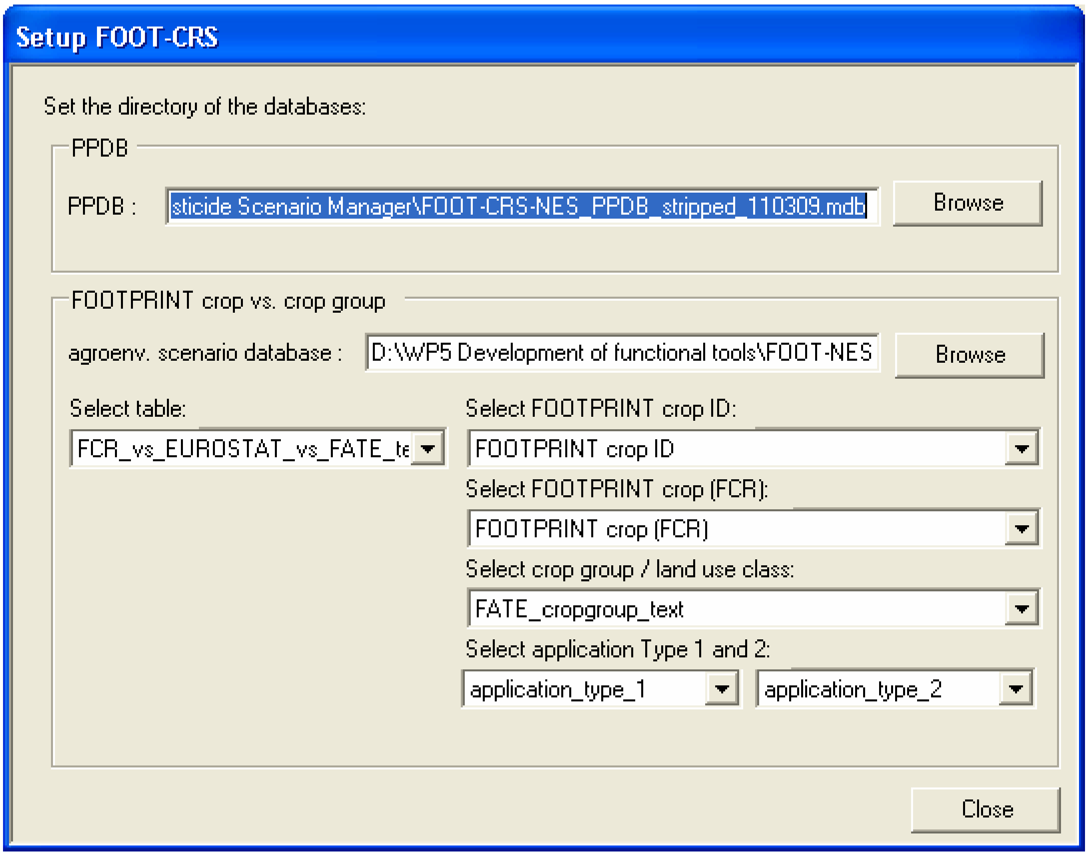


Figure 26 - The Setup window of the FOOT-CRS Pesticide Scenario Manager

The Setup window can also be accessed later by clicking "Setup" on the main window of the Pesticide Scenario Manager (cf. Fig. 27). This is useful since the FOOTPRINT PPDB is continuously updated, and the user might want to switch to a newer version from time to time.

The pesticide application scenarios

In the left part of the Pesticide Scenario Manager main window there is a list of the available pesticide application scenarios. The user can administrate existing scenarios (copy, rename or delete), load an existing scenario and modify it, or create a new scenario.

When the user creates a new pesticide application scenario, he/she has to specify an AOI (= area of interest) shapefile. This can be an agro-environmental scenario shapefile (created with the Data Manager for a given catchment boundary shape) or a subset of it (covering only a subcatchment of the orginal catchment). Creating an AOI shape as a subset of an existing agro-environmental scenario shape is easy: Simply select the polygons of interest in the relevant agro-env. scenario shapefile in ArcGIS and export them as a new shapefile.

Tab Pesticides

In this tab, the user can select/enter the compound to be modelled and its properties. If a compound is selected from the FOOTPRINT Pesticide Properties Database (cf. section 4) in .mdb format, automatically the following fields are filled with values from the PPDB:

- DT50
- K_{oc}
- Degradation half-life in surface water
- Degradation half-life in sediment

These default values can be overwritten by the user. Instead of selecting a compound from the PPDB, the user can also enter an own compound name.

The reference temperature of water/sediment studies is set by default to 20 °C, since this is the usual temperature at which water/sediment studies are conducted in the laboratory. However, the user can also overwrite this value.

In the lower group box of the tab, the user can select drift percentiles for surface water calculations in the listbox “Percentile spray drift”: These percentiles refer to percentiles of the drift percentage distribution of the Rautmann-Ganzelmeier drift trials. This distribution reflects differences in experimental conditions (wind speed, spraying equipment etc.). The X^{th} percentile is defined as the value of a variable that corresponds to a cumulative relative frequency or cumulative probability of X %. That is, a higher percentile corresponds to a worse case and will result in higher pesticide inputs into surface water.
The user can (and has to) select one value.

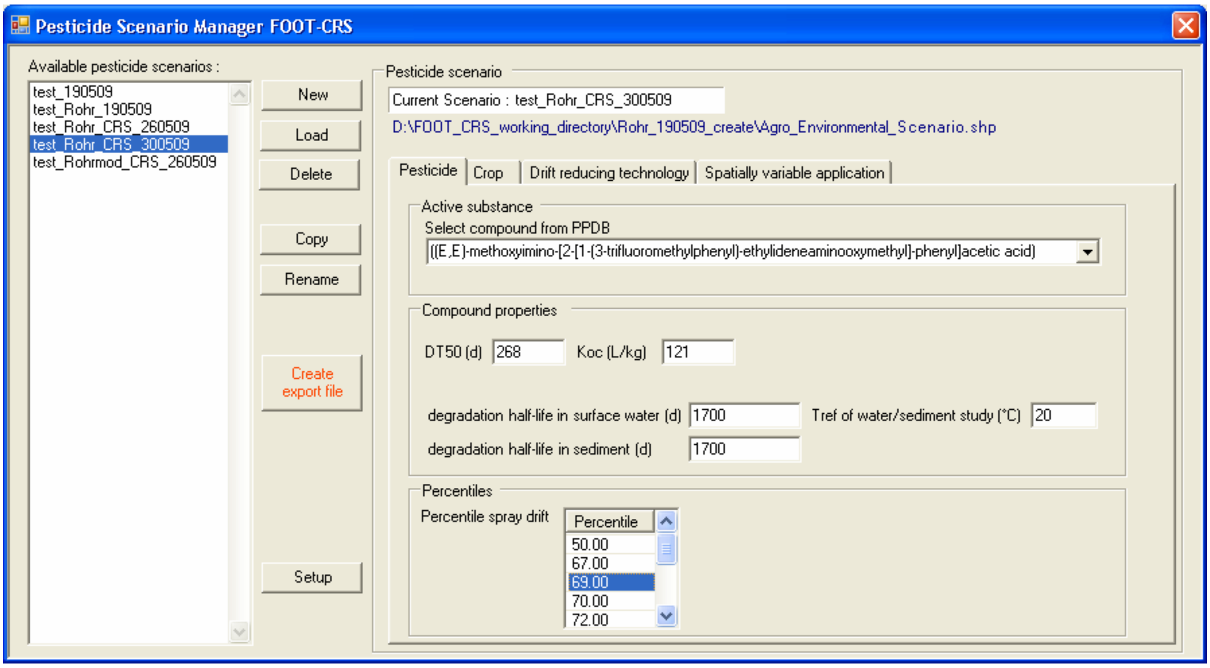


Figure 27 - The FOOT-CRS Pesticide Scenario Manager, Tab "Pesticide"

Tab Crop

In this tab (Fig. 28), the user selects crop(s), application type and distance to the nearest surface water body.

First, the user specifies the number of crops for which applications of the pesticide specified in the previous tab are to be modelled. The user can specify up to 45 crops. Subsequently, a list appears with three columns and as many records as the number of crops specified above. For each record, the user has to fill in all three columns:

- "Crop": The user can select one of 42 available FOOTPRINT crops. If multiple applications to the same crop (e.g. in different months) are to be modelled, the user can select the same crop more than once (cf. the example "spring barley" in Fig. 28).
- "Application type": For arable crops, only "ground spray" is available as application type. For taller permanent crops (pome/stone fruit trees, vines, citrus, olives, hops, bush berries), both "ground spray" (usually for herbicide application) and "air blast" (usually for insecticide and fungicide application) are available.
- "Minimum distance to water body (m)": This is the minimum distance from the edge of the *sprayed* area to the surface water body. In other words, it's the width of a no-spray zone. Hence, it can be used to assess the effect of no-spray zones on pesticide drift inputs into surface waters. Any other drift mitigation is dealt with somewhere else.

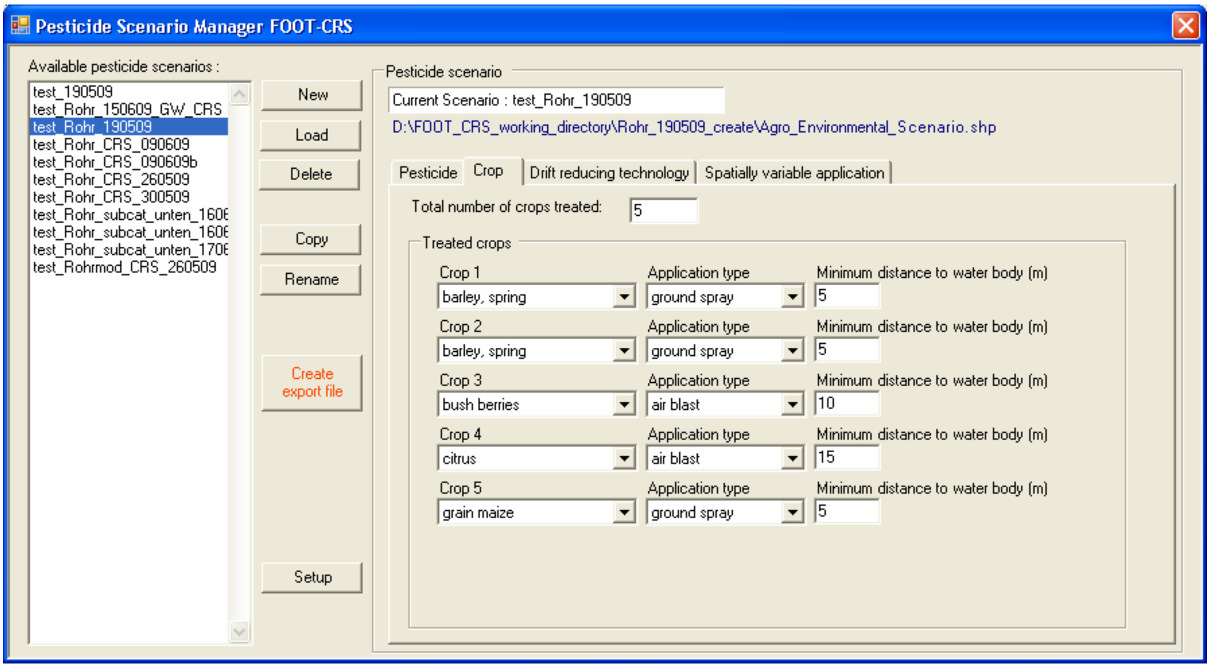


Figure 28 - The FOOT-CRS Pesticide Scenario Manager, Tab "Crop"

Tab Drift reducing technology

In this tab (Fig. 29), the user can specify whether drift mitigation due to drift reducing technology is to be simulated, and how effective the various drift mitigation measures are. The default reduction efficiencies can be overwritten by the user, but it is not possible to obtain an overall mitigation factor due to drift reducing technology < 0.05. That is, it's not possible within the tool to obtain more than 95 % drift reduction by the use of drift reducing technology. This tab is identical to the one in FOOT-NES.

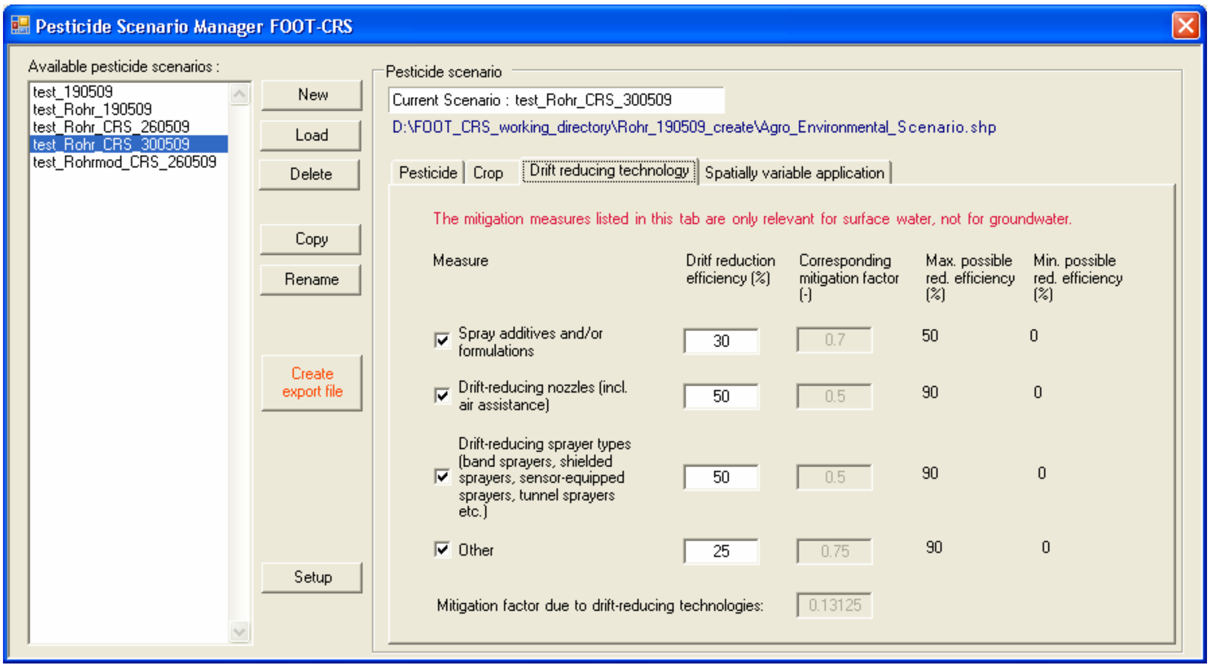


Figure 29 - The FOOT-CRS Pesticide Scenario Manager, Tab "Drift reducing technology"

Tab Spatially variable application

In this tab (Fig. 30), the spatially variable application and mitigation can be launched separately for each crop by clicking "Define", upon which the window "Spatially variable application for selected crop" (see below) opens and a copy of the AOI (area of interest) shapefile is loaded in ArcGIS.

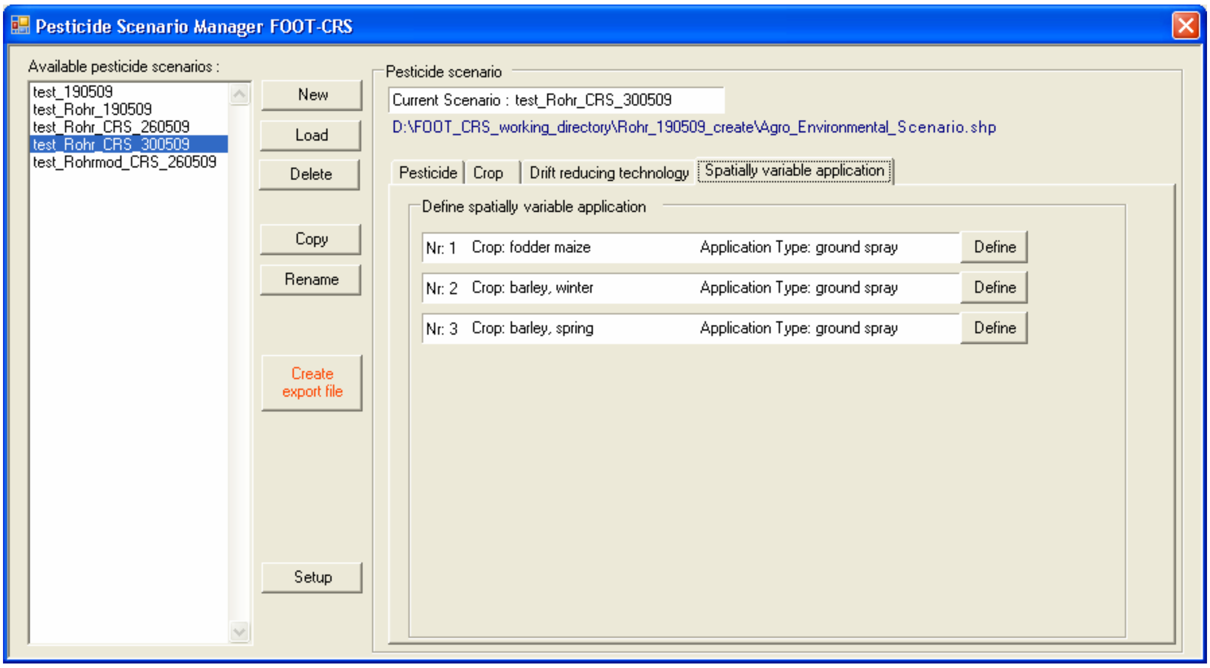


Figure 30 - The FOOT-CRS Pesticide Scenario Manager, Tab "Spatially variable application"

Window "Spatially variable application for selected crop"

In this window (Fig. 31), the spatially variable application is performed for the selected crop (the one for which "Define" was clicked in the tab "Spatially variable application). The course of action is as follows:

1. Select polygons in ArcGIS (cf. Fig. 31)
2. Make the following entries (cf. Fig. 32)
   - application rate (Note: Please enter the actual application rate here, since pesticide interception by the crop is already included in the MACRO and PRZM simulations.)
   - application date (day and month)
   - percentage treated of crop group area (Important: The percentage has to refer to the area of the crop group indicated in green on the window (e.g. barley), not to the area of the FOOTPRINT crop (e.g. winter barley).
3. Click on "Set" (This will write the settings made for the selected polygons into the attribute table of the shapefile.)
4. Repeat steps 1-3 with new polygons
5. When finished, click "Close".

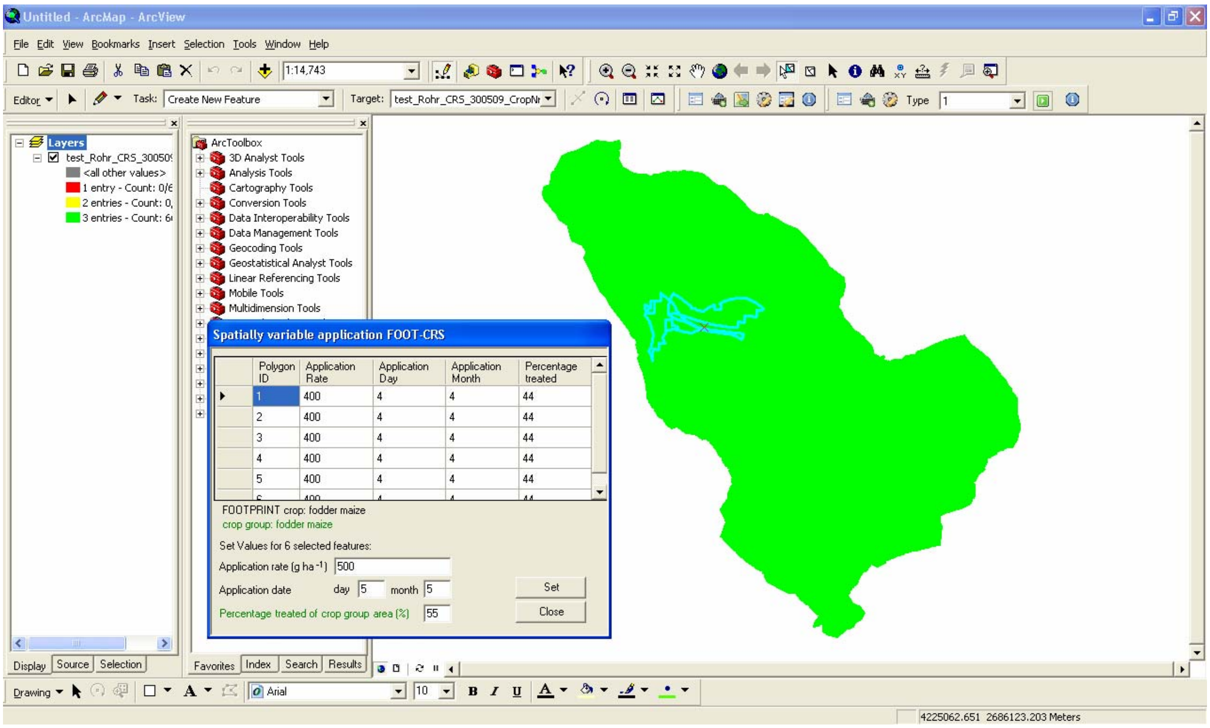


Figure 31 - ArcGIS screen with window "Spatially variable application for selected crop", a copy of the AOI shape and selected polygons

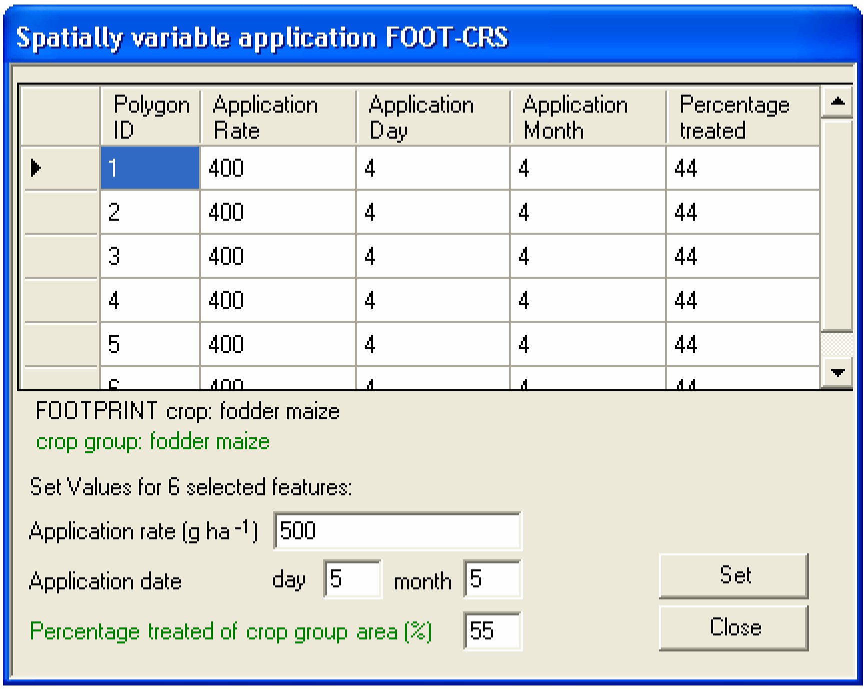


Figure 32 - The FOOT-CRS Pesticide Scenario Manager, Window "Spatially variable application for selected crop"

Exporting the created applications

After filling all tabs and specifying applications in the window “Spatially variable application for selected crop”, the applications specified for the various crops and polygons in the active pesticide application scenario can be exported as a text file (.fps), which is then read by the FOOT-CRS Modelling Module (cf. section 3.1.8).

Note that in FOOT-CRS, for the input pathways runoff/erosion/drainage records are written to the .fps also for non-treated polygons. This is necessary because also non-treated polygons contribute drainflow and surface runoff water.

3.1.6 The Landscape feature digitizer

The landscape feature digitizer allows the user to manually create a landscape feature or mitigation feature shapefile. The procedure is as follows:

1. Create an empty shapefile in ArcGIS
2. Draw polygons of landscape features / mitigation features using the ArcGIS Editor toolbar (usually against the background of an aerial photo or high-resolution satellite image)
3. Select one or more of the freshly drawn polygons and select a landscape feature type (1-6) in the dropdown list of the Landscape feature digitizer (cf. Fig. 33).
4. Assign the landscape feature type to the polygon(s) by clicking the green button right of the list (upon clicking, the selected landscape feature type is written to the records of the selected polygons in the attribute table of the shapefile).
5. Repeat 2.-4. until the landscape feature shapefile is ready

The meaning of the six landscape feature types (Tab. 21) is also given in the Landscape / Mitigation features tab of the FOOT-CRS Data Manager (section 3.1.5).

Landscape feature type (numeric)	Landscape feature type (text)
1	hedge/forest (deciduous)
2	hedge/forest (evergreen)
3	Grass
4	Shrubs
5	inland wetlands
6	maritime wetlands

Table 21 -The FOOTPRINT landscape feature types

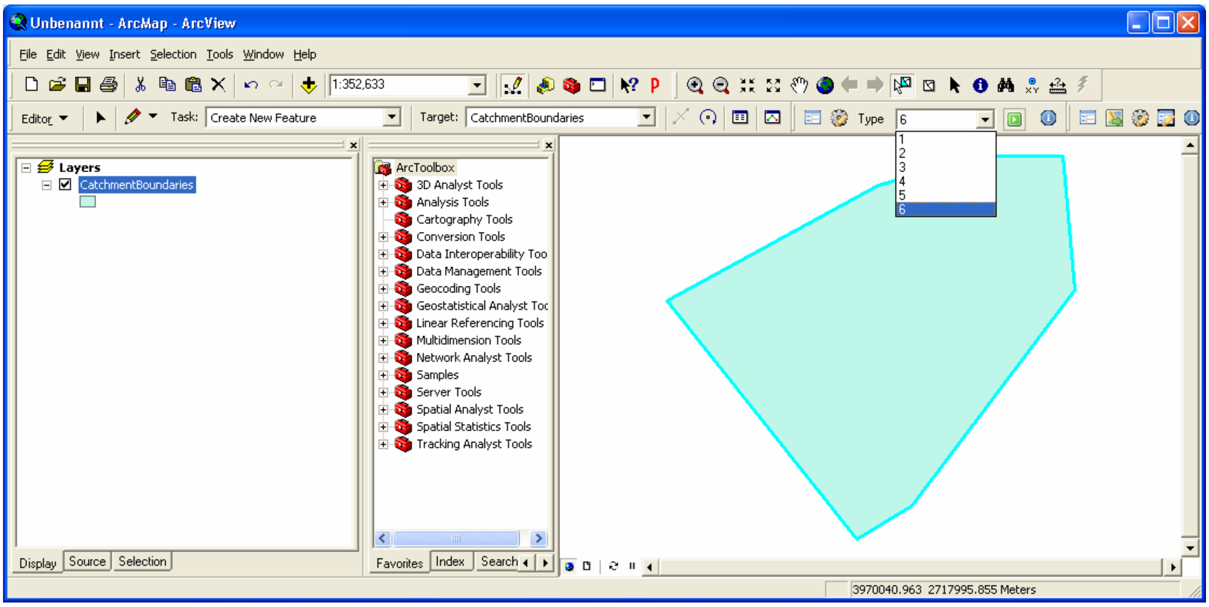


Figure 33 -The Landscape Feature Digitizer

3.1.7 The FOOT-CRS Dominant Pathways Module

So far the Dominant Pathways Module is available only for FOOT-NES (cf. section 3.2.6). The FOOT-CRS Dominant Pathways Module will basically be an upgrade of the FOOT-NES Dominant Pathways Module, since it will consider the presence of landscape features and will perform a surface runoff routing and grid-based drift calculations (cf. DL25; Reichenberger et al., 2008b).

3.1.8 The FOOT-CRS Modelling Module

The FOOT-CRS Modelling Module is only partly available at the moment. While the leaching and drainage calculations are fully functional, the surface runoff and erosion calculations have only partly been implemented so far (the surface runoff routing procedure and the calculation of pesticide inputs into surface water are working, but the PECsw calculation is still being implemented), and the drift calculations are still missing completely.

The FOOT-CRS Modelling Module does the actual pesticide-related calculations in FOOT-CRS. It

- reads and processes the input from the Pesticide Scenario Manager (.fps file and AOI shape)
- accesses the currently active agro-environmental scenario database (as set in the Data Manager)
- extracts values from the various Modelling Databases
- calculates leaching concentrations, pesticide losses from fields, pesticide inputs into the surface water network, and concentrations in surface water at the catchment outlet.
- produces maps and spatial and temporal CDFs (tables and graphs).

The left part of the main window of the Modelling Module (e.g. Fig. 34) lists the available pesticide application scenarios produced by the Pesticide Scenario Manager. The user selects one scenario and checks if he/she wants to both groundwater and surface water calculations, or only one of them. Subsequently, some options have to be set on the tabs “Options Groundwater” and/or “Options Surface Water”.

Tab “Options Groundwater”

This tab is almost identical to its counterpart in FOOT-NES.

- The group box “Spatial aggregation for output as map” (Fig. 34) refers to the method of aggregating PECgw to polygons for map display.
- In the group box “Area for which CDFs are to be produced”, the user chooses whether spatial CDFs of results are to be produced for the whole area of interest (AOI shape) or administrative units of a given level (e.g. NUTS2). The administrative level available for aggregation is NUTS2 for the default agro-environmental scenario database, while for databases created with the Data Manager the available administrative level is the one specified in the Land Cover / Land Use tab of the Data Manager (cf. Section 3.1.4). Consequently, the “NUTS2” entry will soon be renamed to “user-defined administrative units”, and the “NUTS0” entry will be removed from the tab.
- The two options in the group box “CDFs refer to” mean the following:
    - CDFs “whole area”: area % (y-axis) refer to *total* area of the *simulated* crop group(s) (e.g. barley, soft wheat, rye)
    - CDFs “treated area”: area % (y-axis) refer to *treated* area of the *simulated* crop group(s) (e.g. barley, soft wheat, rye)

- Finally, in the group box "Groundwater risk analysis" the user chooses whether a "GW risk map" (a classified PECgw/SUGAR map) shall be produced or not.

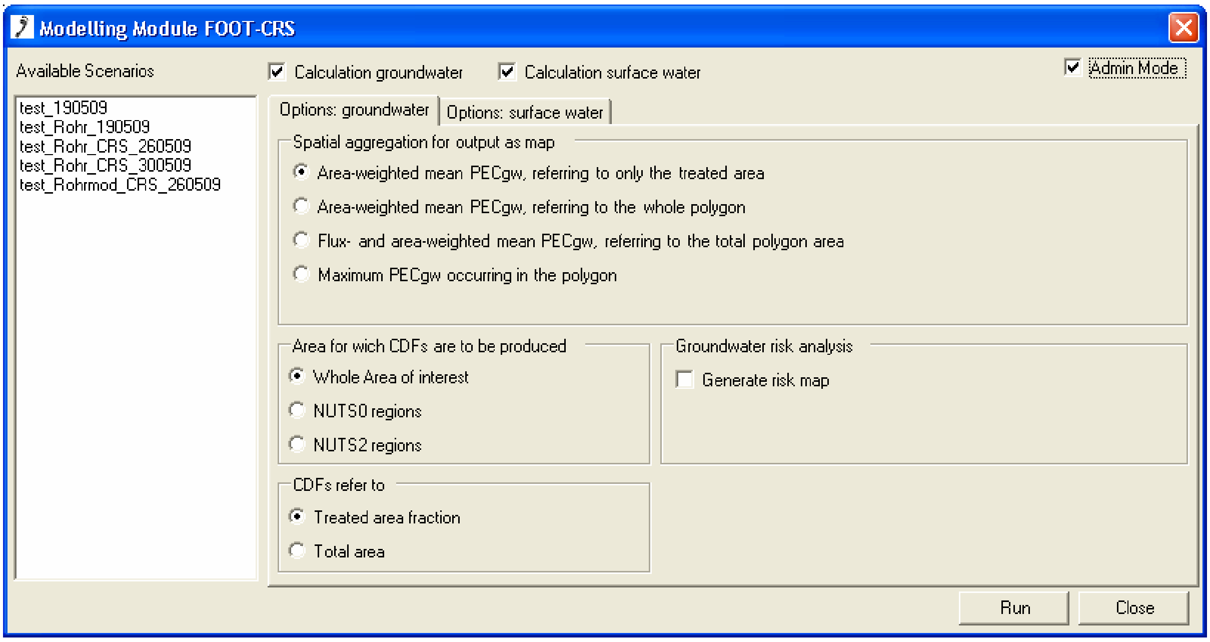


Figure 34 -The FOOT-CRS Modelling Module, Tab "Options Groundwater"

Tab "Options surface water"

Apart from the group boxes with options for spatial aggregation, this tab has two other group boxes (Fig. 35):

- In the group box "Output" the user specifies the desired output variables:
  - Pesticide edge-of-field losses (surface runoff, erosion, drainage, lateral subsurface flow)
  - Pesticide inputs into surface waters (surface, runoff, erosion, drainage, lateral subsurface flow, drift)
  - Predicted Environmental Concentrations (PEC) in surface water at the catchment outlet
- In the group box "PECsw to calculate" the user selects which types of PECsw (representing different input pathways and/or assumptions) shall be calculated
- In the group box "Create maps/CDFs of maximum losses/inputs for each of", the user chooses whether maps/CDFs of maximum pesticide losses from fields and/or pesticide inputs into surface water shall be produced for each of 12 calendar months or each of 20 simulation years. The option "240 simulation months" has been removed because it would lead to an infeasibly large number of maps and CDFs.

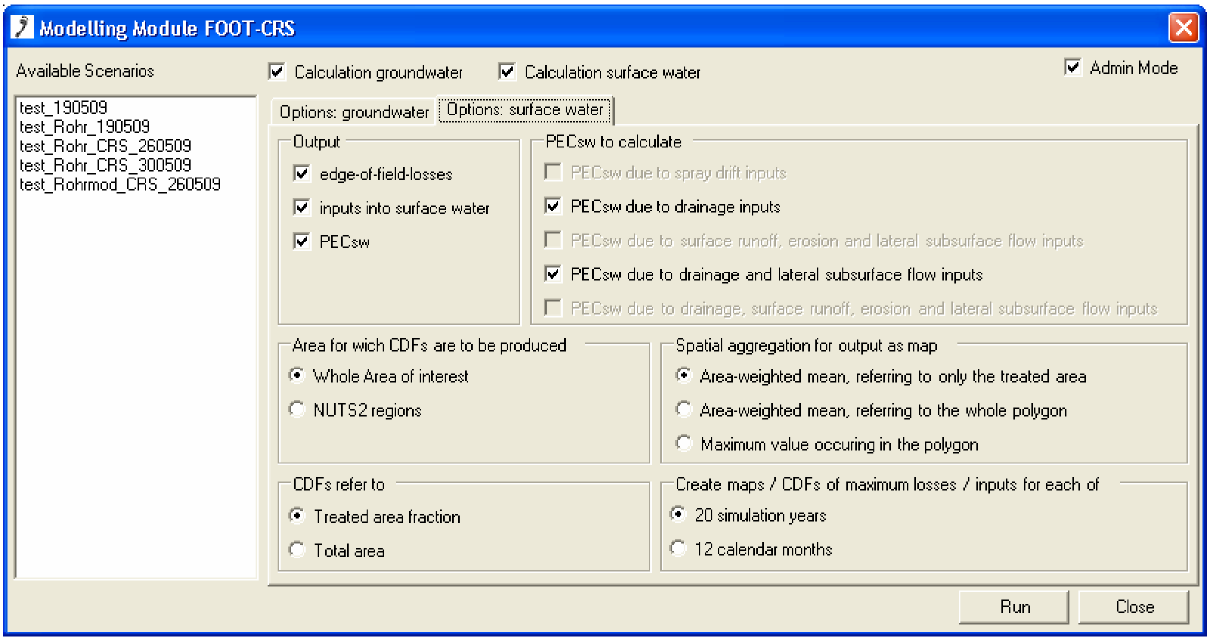


Figure 35 - The FOOT-CRS Modelling Module, Tab "Options Surface water"

Running the Modelling Module

After setting all options in the desired way (cf. Fig. 34 and 35), the user can launch the Modelling Module by clicking on "Run".

The Modelling Module produces

- an output shapefile with the selected output variables as columns in the attribute table
- spatial cumulative distribution functions (CDFs) for the selected loss/input output variables as .dbf tables.
- temporal cumulative distribution functions (CDFs) for the selected PECsw output variables as .dbf tables.
- basic spatial / temporal CDF graphs based on the dbf files mentioned above. These graphs can be accessed in ArcGIS under Tools/Graphs and be saved in different graphics formats. Note that these graphs are only temporary and are lost when closing ArcGIS, unless they have been saved by the user by simply saving the current ArcMap Document (.mxd).
- for each run, a small .txt file that documents the pesticide application scenario used and the options selected.

3.1.9 The FOOT-CRS Communication and Reporting Module

Apart from presenting the results of the Dominant Pathways Module, the task of the Communication and Reporting Module is to display the output variables produced by the Modelling Module (maps, spatial and temporal CDFs). To enable the display of modelling results, the user first has to select in ArcGIS an output shapefile produced by the modelling module.

So far the Communication and Reporting Module is available only for FOOT-NES (cf. section 3.2.8). However, there are only a few minor modifications necessary to adapt the FOOT-NES Communication and Reporting Module to FOOT-CRS:

- Add two tabs (similar to the existing “Table Results” tab in FOOT-NES for spatial CDFs) for the temporal CDFs of PECsw:
  - Tab “PECsw – temporal percentiles”
  - Tab “PECsw for given return periods”
- Add functionality to display the relative importance map for drift (output of FOOT-CRS Dominant Pathways Module)
- Add functionality to display the three optional groundwater-related maps along with the groundwater risk map (PECgw/SUGAR map).

3.2 FOOT-NES

3.2.1 Overview of FOOT-NES (National and EU Scale)

FOOT-NES is a GIS-based tool for pesticide risk assessment at the national and EU scale. It is to be used at the large scale by EU and MS policy- and decision-makers, ministries and pesticide registration authorities. The emphasis in FOOT-NES is on i) identifying the areas most at risk from pesticide contamination and ii) assessing the probability of pesticide concentrations exceeding legal or ecotoxicological thresholds.

Predicted Environmental Concentrations in surface water and sediment (PECsw and PECsed) are calculated for hypothetical edge-of-field water bodies. PECsw and PECsed are calculated for each agro-environmental scenario, and separately for each input path (surface runoff + erosion + interflow; drainage; drift). Finally, PEC for surface water and groundwater are spatially aggregated for display as map and for display as spatial cumulative distribution functions (CDF). With the spatial CDFs of PECsw, the user can e.g. determine the area percentage of exceedance of a given ecotoxicological threshold.

In total, the FOOT-NES modelling module produces the following output for surface water

- Maps and spatial cumulative distribution functions (CDFs) of

  - pesticide losses from fields
  - pesticide inputs into surface water
  - Predicted Environmental Concentrations and Time Weighted Average Concentrations in surface water and sediment (PECsw/sed and TWACsw/sed)

3.2.2 System requirements

To install and run FOOT-NES, the user's system must meet the following requirements:

- OS: Windows XP or Vista (the tool has been developed on XP, but also been tested on Vista)
- Installed software:
  - ArcGIS 9.3
  - ArcGIS .NET Support
  - Microsoft .NET Framework 2.0 or higher
  - Microsoft Access 2003 or 2007
- User account: The user needs admin rights for installation, but not for running the tool

3.2.3 FOOT-NES development

The Pesticide Scenario Manager module has been programmed in VB.NET by David Windhorst (UG) and been extended by the selection and handling of mitigation measures by Moritz Wurm (iNovaGIS). The other modules of FOOT-NES have been developed in the programming language C# ("C sharp") by Björn Feisel (iNovaGIS).

3.2.4 The FOOT-NES Data Manager

The general purpose of the Data Manager is to administrate the input data for the Modelling Module (apart from the pesticide application scenarios) and for the Dominant Pathways Module (cf. Fig. 18). Moreover, it facilitates the import of the user's own data, in case the user wants to replace one or more of the FOOTPRINT default data sets (soil, land cover, land use, etc.) with own datasets. As a consequence of importing one or more user datasets, a new agro-environmental shapefile and database have to be created by the Data Manager.

The FOOT-NES Data Manager is organized in 6 tabs:

- Project
- General
- Land Cover / Land Use Map

- Soil map
- Surface water body characteristics
- Discharge

The currently active settings on all tabs of the Data Manager can be saved as a project. The projects are necessary because the Modelling Module and the Dominant Pathways Module need to know what input data (incl. agroenv. scenario DB and shape) they shall use. That means, when running a pesticide application scenario in the Modelling Module (cf. section 3.2.7), the user must make sure that the AOI (area of interest) shapefile used by the Pesticide Scenario Manager (cf. section 3.2.5) to create the pesticide application scenario matches with the agroenv. scenario database that is currently active in the Data Manager → The right project must be loaded in the Data Manager before starting a run with the Modelling Module.

The FOOT-NES Data Manager is very similar to its counterpart in FOOT-CRS. In fact, both Data Managers are the same piece of software (i.e., they share the same .dll), but adapt their features to the tool in which they are used.

Tab "Project"

This tab (Fig. 36) is the same as in FOOT-CRS, except that no landscape feature / land cover map is generated (because it is not used by FOOT-NES). Here the user can create and administrate projects, and create files required for running a FOOT-NES assessment. If the user saves a project and clicks on "create" on the project tab, the data manager will create a user-defined agro-environmental scenario shapefile (multi-part) and database. Subsequently, the names and paths of the new shapefile and database will appear on the General Tab as currently active agro-environmental scenario shape and database.

To be able to create an agroenvironmental . scenario map and database, the user must have specified the following input data:

- Climate map
- Land cover / land use map (+ assignment performed)
- Soil map and soil table (+ assignment performed)
- discharge

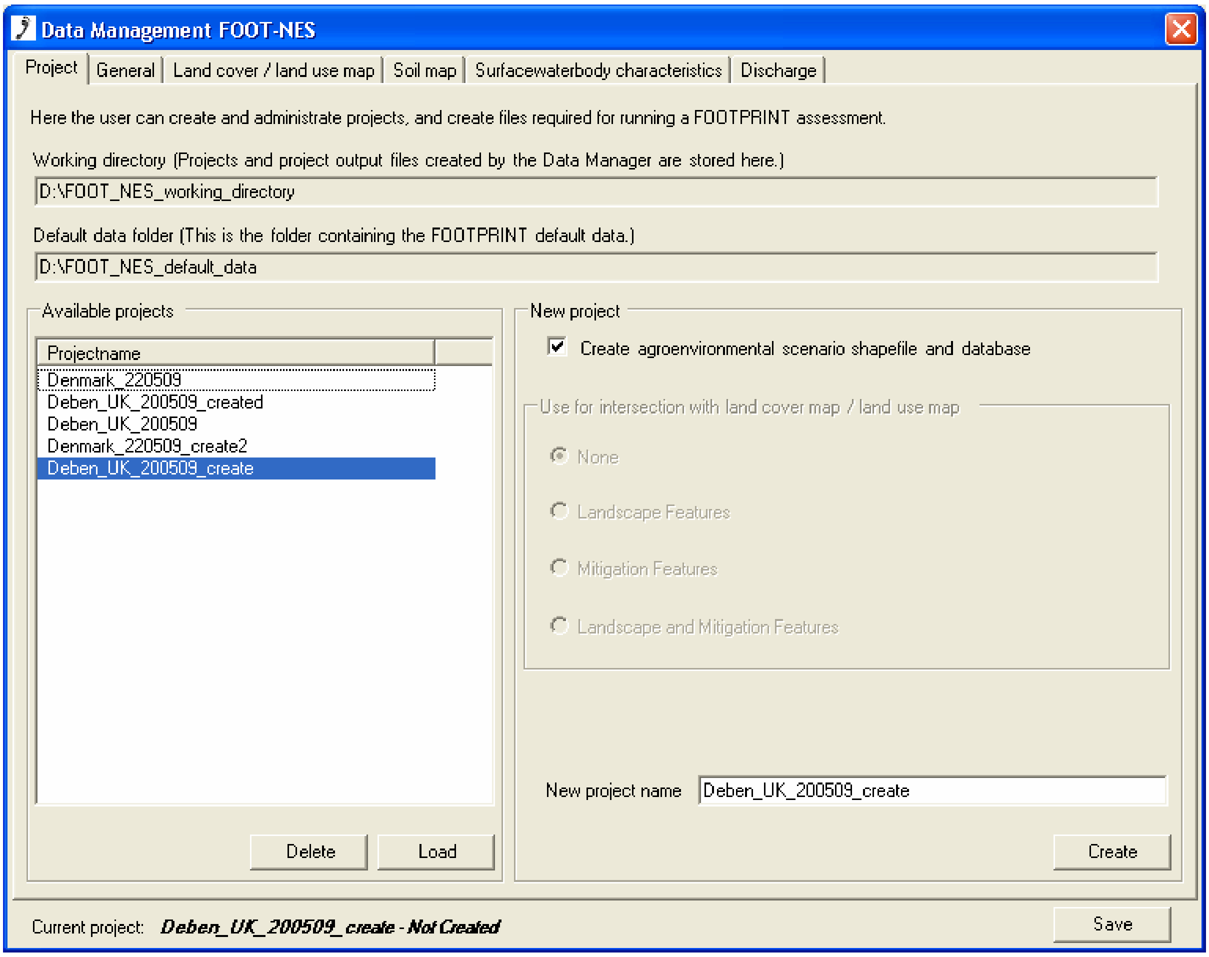


Figure 36 - The FOOT-NES Data Manager, Tab "Project"

Tab "General"

This tab (Fig. 37) is the same as in the FOOT-CRS Data Manager (cf. Feisel et al., 2008), except that no DEM is required and no optional groundwater-related data sets can be specified.

In the "General" tab, the names and paths of various data sets required for creating projects or running an assessment are specified:

- *Default data folder:* This is the folder where the FOOTPRINT default data are stored (this path will become relevant when the final version of FOOT-NES is distributed along with European-level default data sets)
- *Working Directory:* This the folder where the Data Manager stores the files and projects it creates.
- *Agroenvironmental scenario shapefile:* This is the currently active agro-environmental scenario shape, i.e. the one currently to be used by the Dominant Pathways module. It can be either the default or an user-defined agro-environmental scenario shape (depends on

the project).

Note: The modelling does not work with this shape, but with the AOI shape specified in the Pesticide Scenario Manager, which is either an agro-environmental scenario shape or a subset of one.

- *Agroenvironmental scenario database:* This is the currently active agro-environmental scenario database, i.e. the one currently to be used by the Modelling module and the Dominant Pathways module. It can be either the default or an user-defined agro-environmental scenario DB (depends on the project). Note that the active agro-environmental scenario shape and database must match each other.
- *Control modelling database:* This is an Access database which lists the names of the various Modelling databases with MACRO and PRZM results. In more detail, for each crop/climate combination it gives the name of the corresponding gw database, and for each crop/climate combination it gives the name of the corresponding sw database. The control modelling database has to be in the same folder as the Modelling databases.
- *FOOTPRINT climate zones shapefile:* This is the shapefile containing the FOOTPRINT climate zones. It cannot be edited or replaced by the user.
- *SUGAR map:* Map of the FOOTPRINT SUGAR (Surface Water / Groundwater Contribution) Index. This can be the European level default SUGAR map or a more detailed map based on the user's own data.
- *FOOTPRINT classification database:* This database contains the tables to fill the assignment boxes on the Land Cover / Land Use tab, the soil tab and the surface water body characteristics tab.

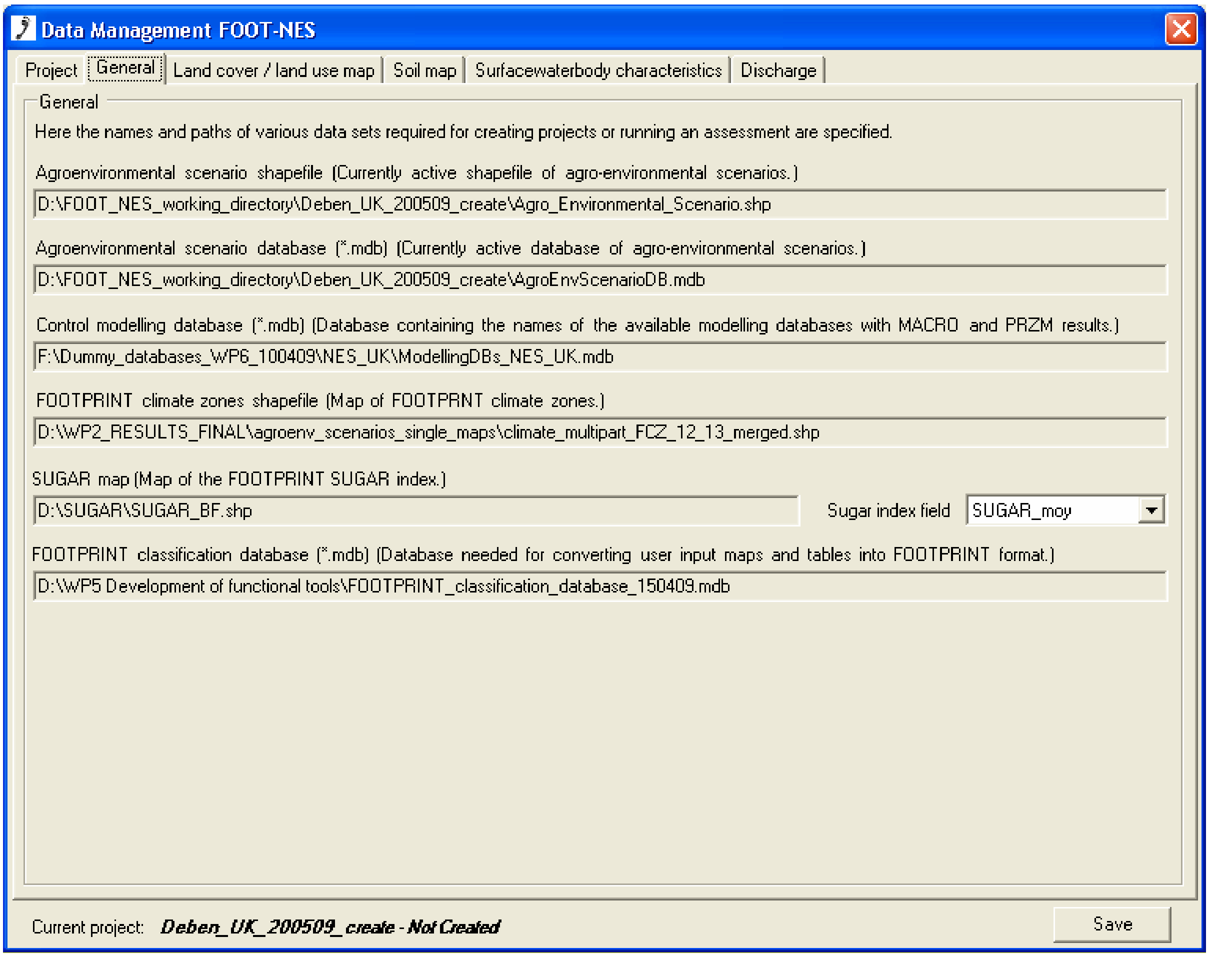


Figure 37 - The FOOT-NES Data Manager, Tab "General"

Tab "Land Cover / Land Use map"

This tab (Fig. 38) is identical to the one in FOOT-CRS, with one exception: In FOOT-NES the user needs to specify two administrative levels. Both levels will be available as aggregation options for pesticide losses, inputs and PEC to CDFs in the FOOT-NES Modelling Module. Before the release of FOOT-NES, the currently displayed names "NUTS0" and "NUTS2" will be renamed to "higher level administrative code field" and "lower level administrative code field", respectively. The reason is that the methodology is generic and not restricted to NUTS0 (EU countries) and NUTS2 (districts, e.g. "Regierungsbezirk" in Germany) levels.

In the Land Cover / Land Use tab, the user can import own land cover and/or land use data in shapefile format (or just specify the default land cover / land use map).

The Land Cover / Land Use map must contain both land cover (type of cover of the soil) and land use (area fractions of crop groups based on agricultural statistics). Consequently, the shapefile the user specifies must contain the following columns (fields) in its attribute table:

- Administrative code field on which the agricultural statistics are based (this administrative level is then available as an aggregation option for pesticide losses and inputs to CDFs in the Modelling Module). It has to be specified in the listbox “NUTS2 code field”.
- Higher-level administrative code field. This level is then also available as an aggregation option in the Modelling Module. It has to be specified in the listbox “NUTS0 code field”.
- The column that contains the land cover classes (e.g. CLC classes). It has to be specified in the listbox “Land Cover Code field”.
- Various columns containing the area fractions of the various crop groups in the polygons of the shapefile (Note that the LC/LU map can be a multi-part or a single-part shapefile; the Data Manager doesn’t mind either format. But the user must decide before creating his/her LC/LU shapefile which format is more appropriate for his/her purpose!)

In the group box “Land Cover”, the user can assign FOOTPRINT land cover codes (CORINE Land Cover format) (e.g. 211 = “non-irrigated arable land”) to the land cover codes of his/her own map LC/LU map. If the user’s land cover codes are already in CLC format (as is the case for the default LC/LU map), an automatic assignment can be performed by clicking on the text “automatic assignment”.

In the group box “Land Use”, the user can assign FATE crop groups or land use classes (e.g. VALUE_72 = barley) to the land use classes of his/her own LC/LU map. If the user’s land cover codes are already in FATE format (as is the case for the default LC/LU map), an automatic assignment can be performed by clicking on the text “automatic assignment”.

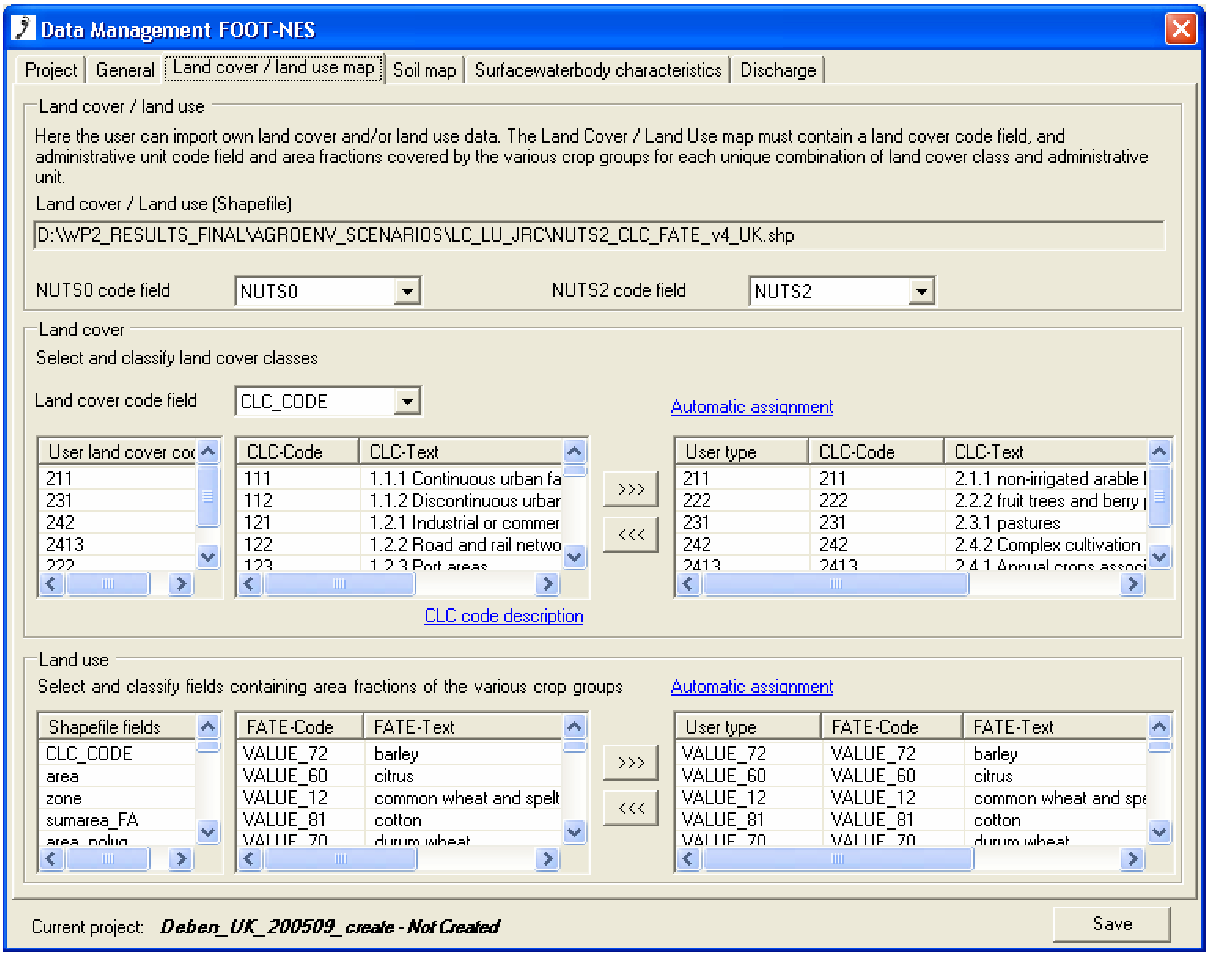


Figure 38 - The FOOT-NES Data Manager, Tab "Land Cover / Land Use map"

Tab "Soil map"

This tab (Fig. 39) is identical to its counterpart in FOOT-CRS. In the tab "Soil map", it the user can import own soil data (or just specify the default soil map and table). The user has to specify both a soil map (shapefile) AND a soil table (.dbf).

The map (shapefile) must contain a column with the soil mapping units (SMU).

The soil table (.dbf) must contain these columns:

- Soil Mapping Unit (SMU) (which must have the same SMU codes as the SMU column in the soil shapefile)
- Soil Typological Unit (STU)
- The area fraction covered by each STU occurring in an SMU.

Note: Usually an SMU contains more than one STU. If, however, there is only one STU per SMU (might occur in detailed user soil maps), the area fraction covered by this STU is 1. However, even is there is only one STU per SMU, the soil table must be physically different from the attribute table of the soil shapefile.

In the lower part of the tab the user can assign FOOTPRINT soil types (FST) and Flow Pathway Categories (FPC) to his/her own STUs, both manually and automatically.

Since in the case of manual assignment the user will usually not know the FST corresponding to his/her STU beforehand, a link will be placed on the tab that opens the FOOTPRINT soil selector software.

Analogously to the land cover / land use tab, there is also an automatic assignment in place, for the case that the user’s soil types are already in FST format. To enable an automatic assignment, the user must specify an FST column and an FPC column in his/her soil table. To increase the performance (calculation speed) of the automatic assignment procedure, it is possible that the file format of the soil table will be changed from .dbf to .mdb before the release of FOOT-NES to the public.

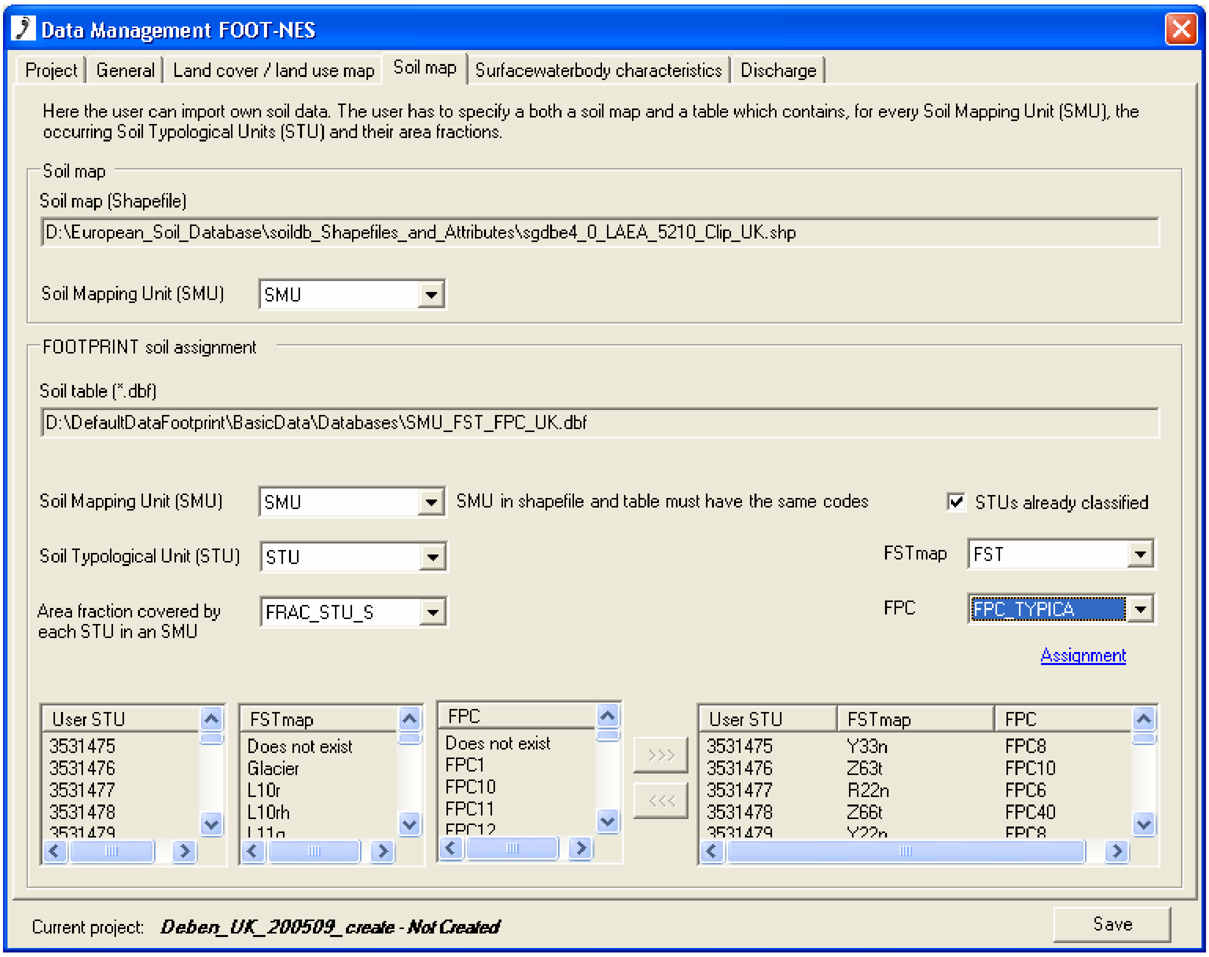


Figure 39 - The FOOT-NES Data Manager, Tab "Soil map"

Tab "Surface water body characteristics"

This tab (Fig. 40) is completely different from the tab "Surface water network" in FOOT-CRS. The reason is that FOOT-NES uses hypothetical edge-of-field surface water bodies as opposed to an observed surface water network.

In this tab, the user can specify characteristics of the hypothetical surface water bodies (ditch, stream and pond). The default values, which were adopted from the FOCUS surface scenarios (FOCUS, 2001), can be overwritten. Moreover, a routine to estimate sediment porosity from bulk density and OC content has been formulated and will be implemented before the release.

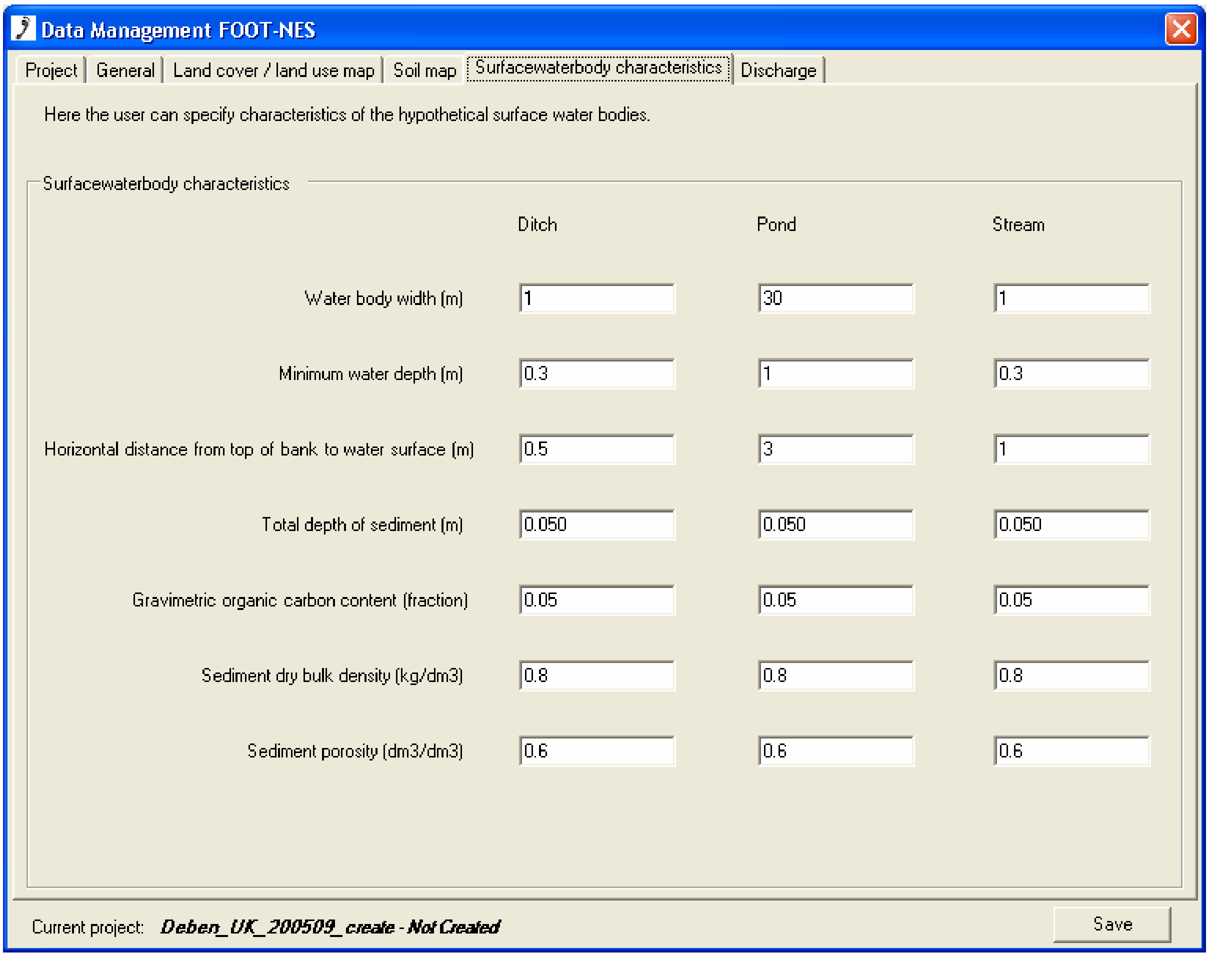


Figure 40 - The FOOT-NES Data Manager, Tab “Surface water body characteristics”

Tab "Discharge"

The tab (Fig. 41) is identical to the discharge tab in FOOT-CRS (cf. section 3.1.4). However, there is an important issue regarding the input data: It must be considered that the FOOT-NES users (in contrast to the FOOT-CRS users) will not necessarily have the Spatial Analyst extension for ArcGIS, which is a lot more expensive than ArcGIS itself. Without this extension, one basically cannot do any raster calculations in ArcGIS. Thus, without the Spatial Analyst, discharge data in form of grids cannot be processed. For this reason, we set up a vector-based methodology for discharge processing in FOOT-NES as a workaround, which has not been implemented yet, but will become available until the release of FOOT-NES. As a consequence, in the final version v.1 there will be two possibilities for the user to specify discharge data:

a) Discharge grids. These are later processed using the zonal statistics function, which works only if the Spatial Analyst extension is installed and active.
b) A shapefile with 12 discharge columns as attributes. The vector-based analogue to the "zonal statistics" function will work also without Spatial Analyst.

In the discharge tab, the user has to specify maps of mean discharge for each calendar month (or just specify the default discharge maps (UNH Composite Runoff Fields; Fekete et al., 2000)). Note that not maps of actual river discharge (in e.g. m^3d^{-1}) are required, but maps of area-specific discharge, i.e. excess water from a unit area that runs off to rivers (mm d^{-1}), e.g. calculated from a climatic water balance.

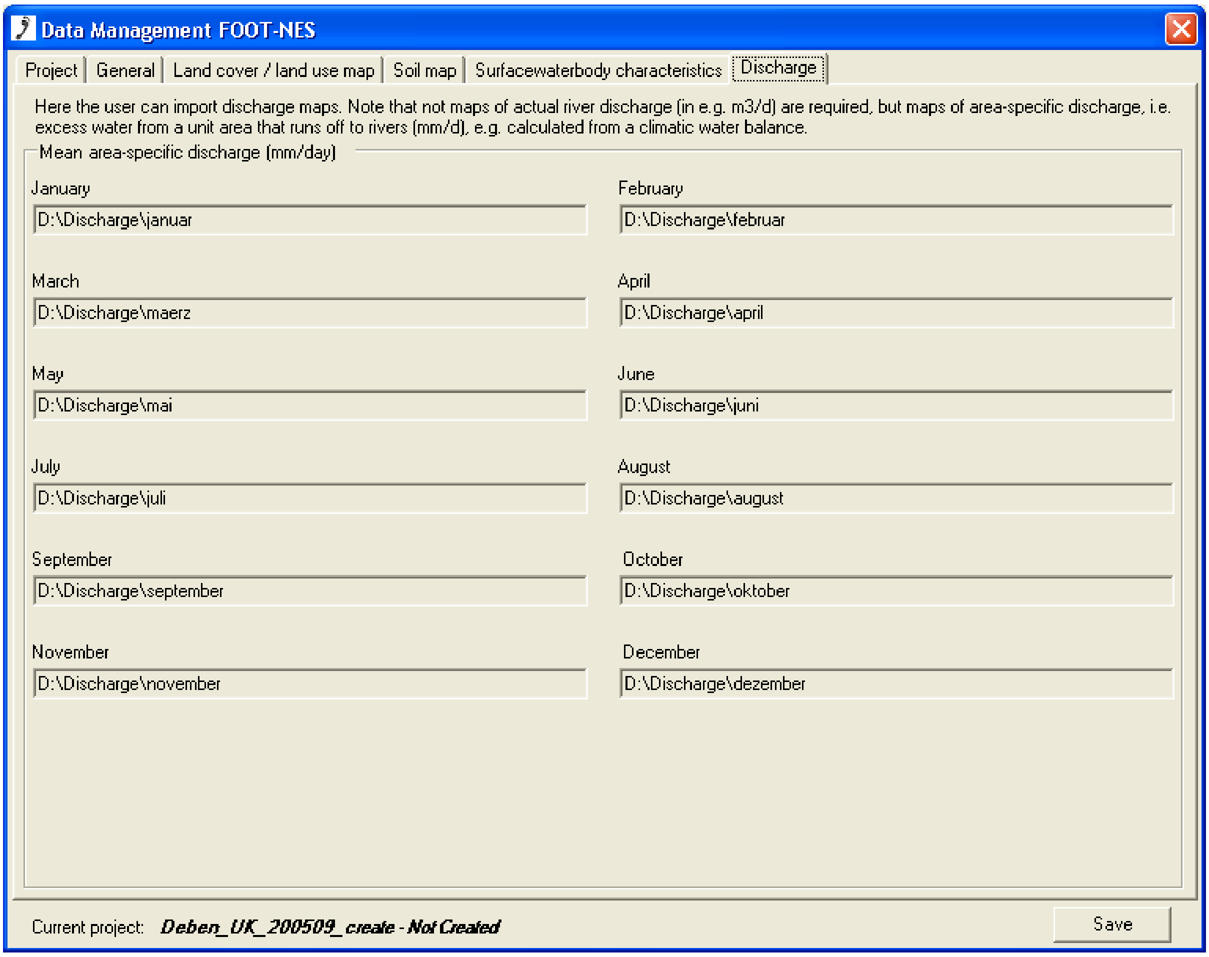


Figure 41 - The FOOT-NES Data Manager, Tab "Discharge"

3.2.5 The FOOT-NES Pesticide Scenario Manager

In this module, the user specifies the pesticide application(s) to be simulated. The module also allows to explore the effects of mitigation (= risk reduction) measures.

The Pesticide Scenario Manager has recently been integrated into the FOOT-NES and FOOT-CRS toolbars and is now included in the combined FOOT-NES/-CRS installation package. The FOOT-NES and FOOT-CRS Pesticide Scenario Managers are the same piece of software, but dynamically adapt their features to the tool in which they are used.

Setting up the Pesticide Scenario Manager

When opening the Pesticide Scenario Manager the first time, the user is prompted to make some settings in the Setup window (cf. Fig. 42):

- Specify the path and filename of the version of the Pesticide Properties Database (PPDB; Lewis et al., 2007) to be used.

- Specify the path and filename of the agro-environmental scenario database to be used. In fact, the Pesticide Scenario manager uses only one table in the agro-environmental scenario database, and this table is also the same in all agro-environmental databases. For convenience of the user, the selection under "select table" jumps automatically to this table ("FCR_vs_EUROSTAT_vs_FATE_text_num"). However, the selections of the right columns in this table have to be done manually exactly according to Fig. 42. The table "FCR_vs_EUROSTAT_vs_FATE_text_num" contains the relations between the 42 FOOTPRINT crops (which are being modelled) and the FATE crop groups (for which there are area fractions contained in the agro-environmental scenario database), and the available application types for each FOOTPRINT crop.

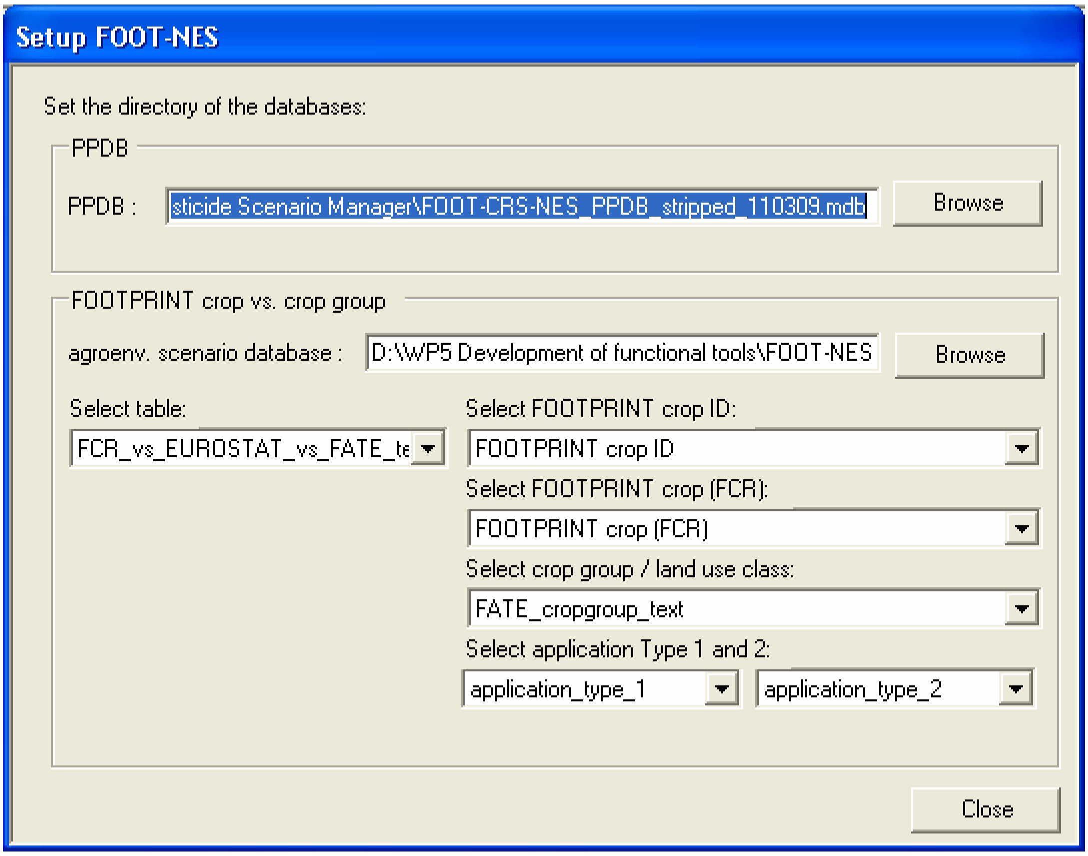


Figure 42 - The Setup window of the FOOT-NES Pesticide Scenario Manager

The Setup window can also be accessed later by clicking "Setup" on the main window of the Pesticide Scenario Manager (cf. Fig. 43). This is useful since the FOOTPRINT PPDB is being continuously updated, and the user might want to switch to a newer version from time to time.

The pesticide application scenarios

In the left part of the Pesticide Scenario Manager main window there is a list of the available pesticide application scenarios. The user can administrate existing scenarios (copy, rename or delete), load an existing scenario and modify it, or create a new scenario.
When the user creates a new pesticide application scenario, he/she has to specify an AOI (= area of interest) shapefile. This can be an agro-environmental scenario shapefile (either the default one or one created with the Data Manager) or a subset of it (i.e. covering only a part of the area of the original agro-environmental scenario shape): If only pesticide applications in a particular country are to be simulated, it would not be too useful to choose an AOI shape covering the whole of Europe, since this would unnecessarily increase calculation times and consumption of storage space. Creating an AOI shape as a subset of an existing agro-environmental scenario shape is easy: Simply select the polygons of interest in the relevant agro-env. scenario shapefile in ArcGIS (e.g. by hand or by using "Select by attribute") and export them as a new shapefile.

Tab "Pesticides"

In this tab (Fig. 43), the user can select/enter the compound to be modelled and its properties. If a compound is selected from the FOOTPRINT Pesticide Properties Database (cf. section 4 of this chapter), automatically the following fields are filled with values from the PPDB:

- DT50
- K_{oc}
- Degradation half-life in surface water
- Degradation half-life in sediment

These default values can be overwritten by the user. Instead of selecting a compound from the PPDB, the user can also enter an own compound name.

The reference temperature of water/sediment studies is set by default to 20 °C, since this is the usual temperature at which water/sediment studies are conducted in the laboratory. However, the user can also overwrite this value.

In the lower group box of the tab, the user can select percentiles for surface water calculations. There are two different lists of percentiles:

- List "Percentile spray drift": These percentiles refer to percentiles of the drift percentage distribution of the Rautmann-Ganzelmeier drift trials. This distribution reflects differences in experimental conditions (wind speed, spraying equipment etc.). The X^{th} percentile is defined as the value of a variable that corresponds to a cumulative relative frequency or cumulative probability of X %. That is, a higher percentile corresponds to a worse case and will result in higher pesticide inputs into surface water.

The user can (and has to) select one value.

- List "Percentile(s) drainage, runoff and erosion": These percentiles refer to the 20-year simulation time series produced by MACRO (drainage) and PRZM (surface runoff and erosion). The X^{th} percentile is defined as the value of a variable that corresponds to a cumulative relative frequency or cumulative probability of X %. That is, a higher percentile corresponds to a worse case and will result in higher pesticide inputs into surface water. Each percentile of the MACRO/PRZM time series directly corresponds to a certain return period (Table 22). If an event has a return period of 10 days, it means that an event of this size will occur on average every 10 days. Note that the higher the percentile is, the more uncertain is the return period.

  The user can (and has to) select one to 11 values.

Percentile	Return period
90.00	10 days
95.00	20 days
96.66	30 days
98.00	50 days
98.67	75 days
99.00	100 days
99.33	ca. 150 days
99.49	ca. 200 days
99.73	1 year
99.90	ca. 3 years
99.97	ca. 10 years

Table 22 -List of percentiles of the MACRO and PRZM time series available in FOOT-NES, and their corresponding return periods

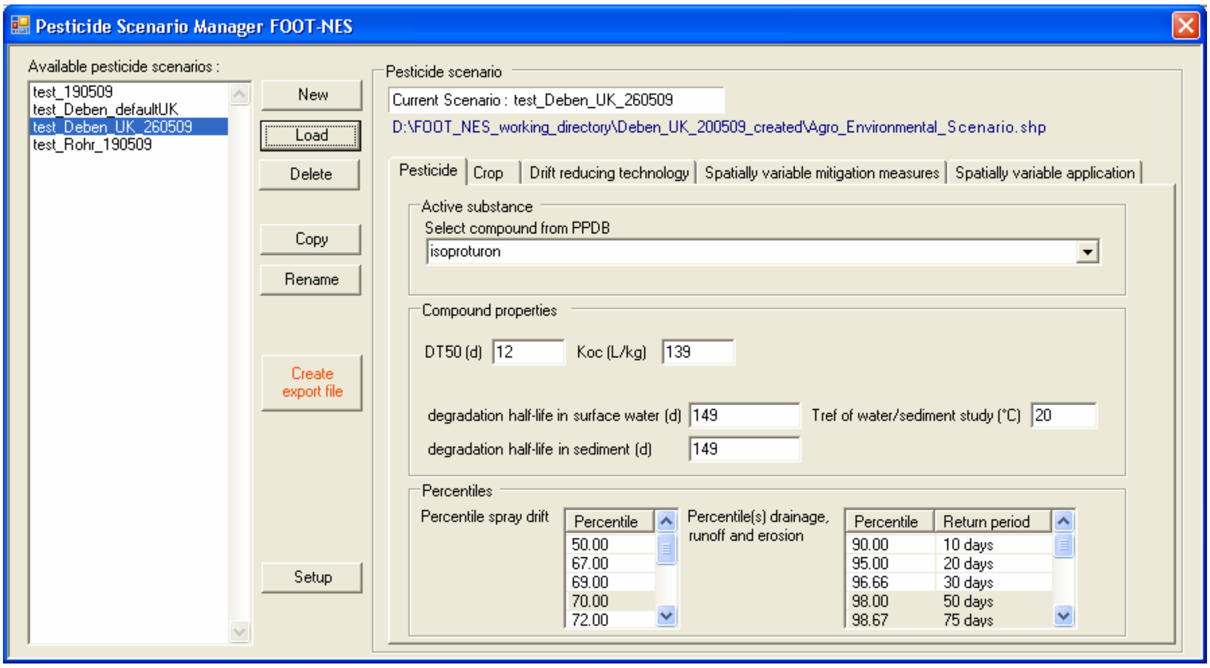


Figure 43 - The FOOT-NES Pesticide Scenario Manager, Tab "Pesticide"

Tab "Crop"

In this tab (Fig. 44), the user selects crop(s), application type and distance to the nearest surface water body. First, the user specifies the number of crops for which applications of the pesticide specified in the previous tab are to be modelled. The user can specify up to 45 crops. Subsequently, a list appears with three columns and as many records as the number of crops specified above. For each record, the user has to fill in all three columns:

- "Crop": The user can select one of 42 available FOOTPRINT crops. If multiple applications to the same crop (e.g. in different months) are to be modelled, the user can select the same crop more than once (cf. the example "spring barley" in Fig. 44).
- "Application type": For arable crops, only "ground spray" is available as application type. For taller permanent crops (pome/stone fruit trees, vines, citrus, olives, hops, bush berries), both "ground spray" (usually for herbicide application) and "air blast" (usually for insecticide and fungicide application) are available.

- "Distance to top of water body bank (m)": This is the distance from the edge of the *sprayed* area to the top of the bank of the surface water body. It is only used for drift input calculation. This distance can be the distance from the actual edge of the field to the water body bank or reflect a no-spray zone. Hence, it can be used to assess the effect of no-spray zones on pesticide drift inputs into surface waters. Any other drift mitigation is dealt with somewhere else.

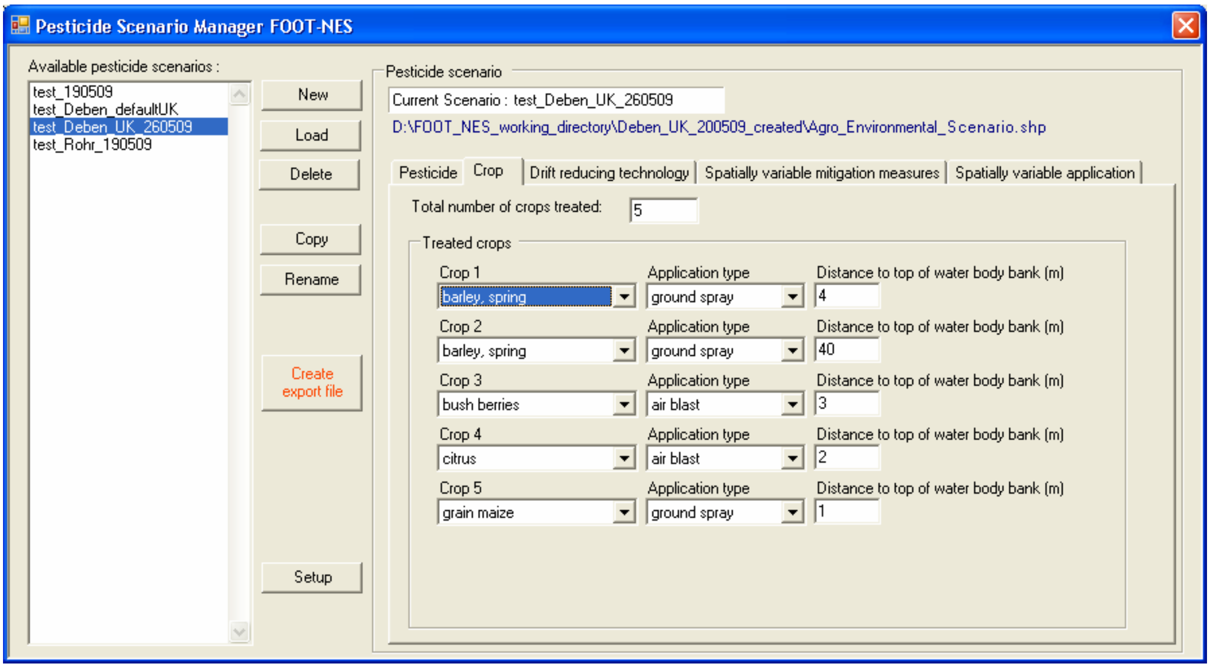


Figure 44 - The FOOT-NES Pesticide Scenario Manager, Tab "Crop"

Tab "Drift reducing technology"

In this tab (Fig. 45), the user can specify whether drift mitigation due to drift reducing technology is to be simulated, and how effective the various drift mitigation measures are. The default reduction efficiencies can be overwritten by the user, but it is not possible to obtain an overall mitigation factor due to drift reducing technology < 0.05. That is, it's not possible within the tool to obtain more than 95 % drift reduction by the use of drift reducing technology. This tab is identical to the one in FOOT-CRS.

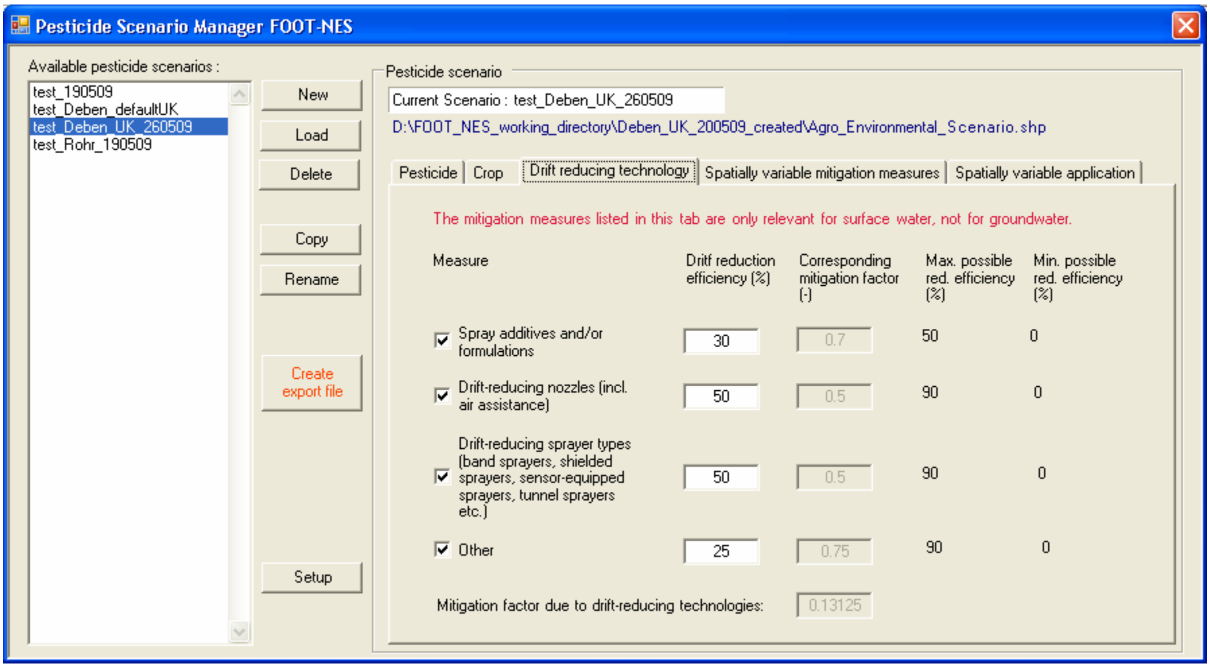


Figure 45 - The FOOT-NES Pesticide Scenario Manager, Tab "Drift reducing technology"

Tab "Spatially variable mitigation measures"

In this tab (Fig. 46), the user can select, for the different crops, further mitigation measures to reduce pesticide inputs into surface waters can be specified in a spatially variable way (i.e. such that they occur in some areas, but not in others, or that they occur with dimensions differing between areas). The available mitigation measures are:

- Riparian buffer strips and hedges
- Grassed edge-of-field buffer strips
- Grassed waterways
- Constructed wetlands

While "riparian buffer strips and hedges" act both as drift mitigation measures and, to a lesser extent, as surface runoff and erosion mitigation measures, the other three act exclusively as runoff and erosion mitigation measures.

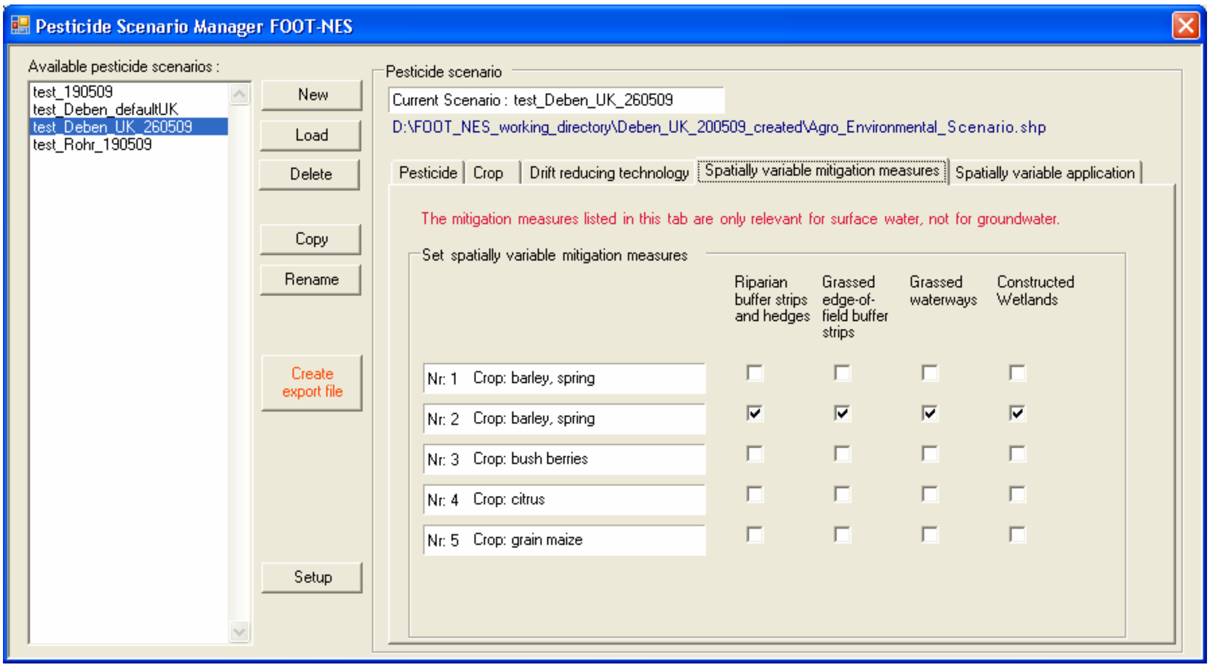


Figure 46 - The FOOT-NES Pesticide Scenario Manager, Tab “Spatially variable mitigation measures”

Tab “Spatially variable application”

In this tab (Fig. 47), the spatially variable application and mitigation can be launched separately for each crop by clicking “Define”, upon which the window “Spatially variable application and mitigation for selected crop” opens and a copy of the AOI (area of interest) shapefile is loaded in ArcGIS.

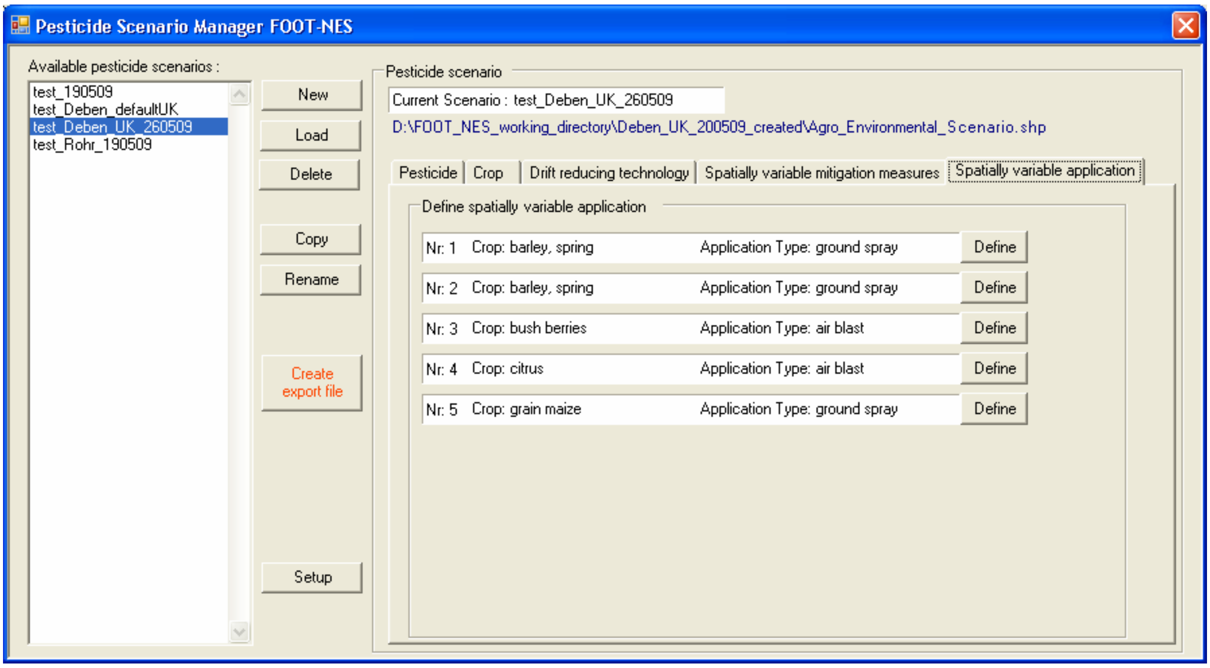


Figure 47 -The FOOT-NES Pesticide Scenario Manager, Tab “Spatially variable application”

Window "Spatially variable application and mitigation for selected crop"

In this window (Fig. 49), the spatially variable application and mitigation is performed for the selected crop (the one for which "Define" was clicked in the tab "Spatially variable application"). The course of action is as follows:

1. Select polygons in ArcGIS (cf. Fig 48)
2. Make the following entries (cf. Fig. 49)
   - application rate
   - application date (Note: Please enter the actual application rate here, since pesticide interception by the crop is already included in the MACRO and PRZM simulations.)
   - percentage treated of crop group area (Important: The percentage has to refer to the area of the crop group indicated in green on the window (e.g. barley), not to the area of the FOOTPRINT crop (e.g. winter barley).
   - If spatially variable mitigation measures have been selected on the tab "Spatially variable mitigation measures", fill in the corresponding fields in the group box "Spatially variable mitigation measures"
3. Click on "Calculate final mitigation factors"
4. Click on "Set" (This will write the settings made for the selected polygons into the attribute table of the shapefile.)
5. Repeat steps 1-4 with new polygons
6. When finished, click "Close".

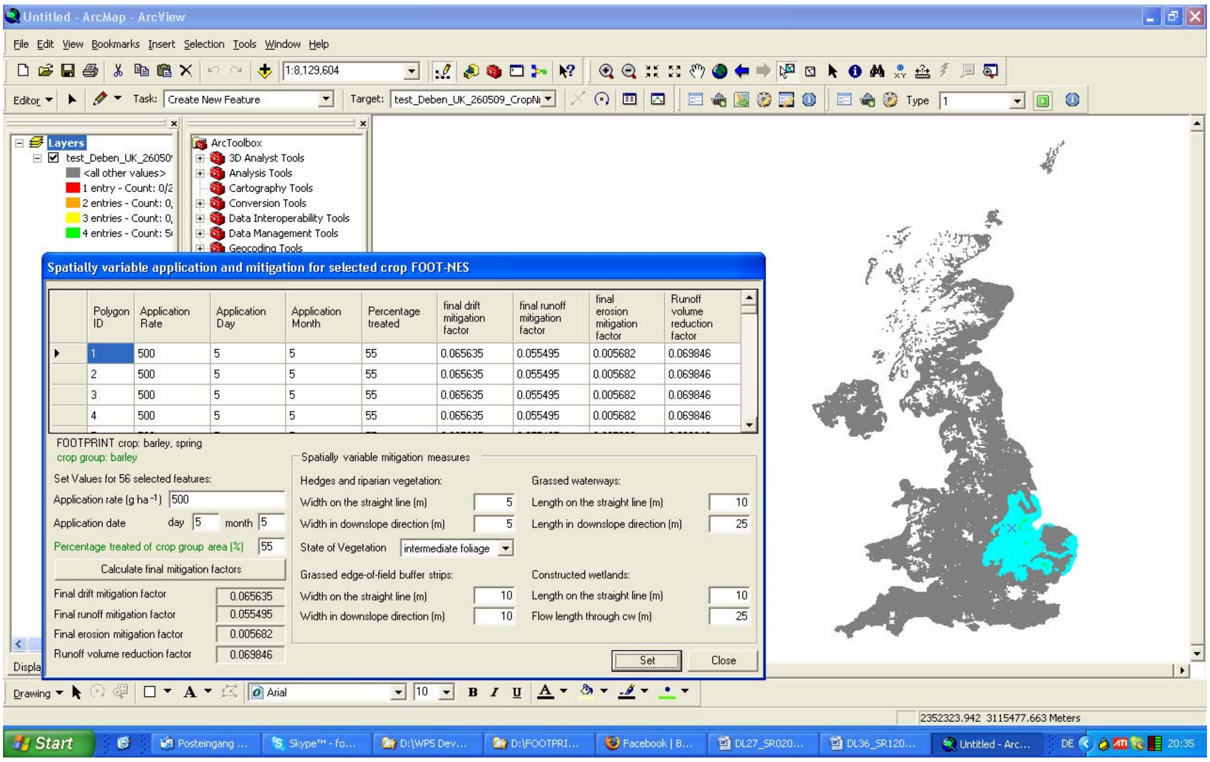


Figure 48 - ArcGIS screen with window "Spatially variable application and mitigation for selected crop", a copy of the AOI shape and selected polygons

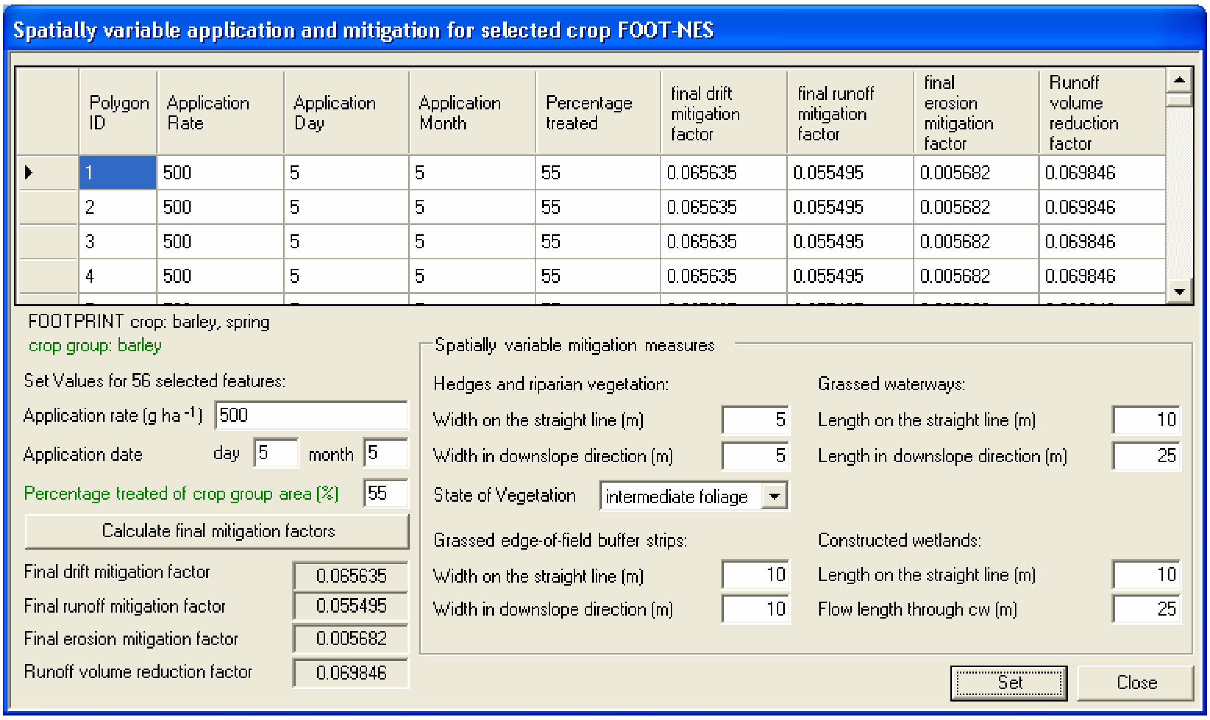


Figure 49 - The FOOT-NES Pesticide Scenario Manager, Window "Spatially variable application and mitigation for selected crop"

Exporting the created applications

After filling all tabs and specifying applications in the window “Spatially variable application and mitigation for selected crop”, the applications specified for the various crops and polygons in the active pesticide application scenario can be exported as a text file (.fps), which is then read by the FOOT-NES Modelling Module (cf. section 3.2.7).

3.2.6 The FOOT-NES Dominant Pathways Module

This module produces maps of the relative importance of the different soil-related contamination pathways, and also a map giving the dominant contamination pathway for each polygon. The final output of the procedure is a set of maps, which can be displayed in colour-coded form by the Communication and Reporting Module (cf. section 3.2.8). The Dominant Pathways Module produces one shapefile with 10 attributes.

The first 8 attributes are the maps of relative importance of contamination pathways for 2 seasonal conditions. This comprises the pathways

- drainage (area-weighted classes based on Flow Pathway Categories FPC)
- surface runoff (area-weighted classes based on FPC)
- erosion (area-weighted classes based on FPC)
- leaching (area-weighted classes based on FOOTPRINT soil types FST, FPC and the SUGAR index)

The other two attributes are maps of dominant contamination pathways for 2 seasonal conditions. These maps indicate the contamination pathways with the highest relative importance for a given polygon.

Since the maps produced by the Dominant Pathways Module are only based on soil properties and the SUGAR index and are independent of pesticide applications, they can also be used as vulnerability maps.

3.2.7 The FOOT-NES Modelling Module

The FOOT-NES Modelling Module does the actual pesticide-related calculations in FOOT-NES. It

- reads and processes the input from the Pesticide Scenario Manager (.fps file and AOI shape)
- accesses the currently active agro-environmental scenario database (as set in the Data Manager)

- extracts values from the various Modelling Databases
- calculates leaching concentrations, pesticide losses from fields, pesticide inputs into surface water bodies, and pesticide concentrations in surface water and sediment.
- produces maps and spatial CDFs (tables and graphs).

The left part of the main window of the Modelling Module (e.g. Fig. 50) lists the available pesticide application scenarios produced by the Pesticide Scenario Manager. The user selects one scenario and checks if he/she wants to both groundwater and surface water calculations, or only one of them. Subsequently, some options have to be set on the tabs “Options Groundwater” and/or “Options Surface Water”.

Tab “Options Groundwater”

- The group box “Spatial aggregation for output as map” (Fig. 50) refers to the method of aggregating PECgw to polygons for map display.
- In the group box “Area for which CDFs are to be produced”, the user chooses whether spatial CDFs of results are to be produced for the whole area of interest (AOI shape), higher-level administrative units (e.g. NUTS0) or lower-level administrative units (e.g. NUTS2). The administrative levels available for aggregation are NUTS0 and NUTS2 for the default agro-environmental scenario database, while for databases created with the Data Manager the available administrative levels are those specified in the Land Cover / Land Use tab (cf. Section 3.2.4)
- The two options in the group box “CDFs refer to” mean the following:
  - CDFs “whole area”: area % (y-axis) refer to *total* area of the *simulated* crop group(s) (e.g. barley, soft wheat, rye)
  - CDFs “treated area”: area % (y-axis) refer to *treated* area of the *simulated* crop group(s) (e.g. barley, soft wheat, rye)
- Finally, in the group box “Groundwater risk analysis” the user chooses whether a “GW risk map” (a classified PECgw/SUGAR map) shall be produced or not.

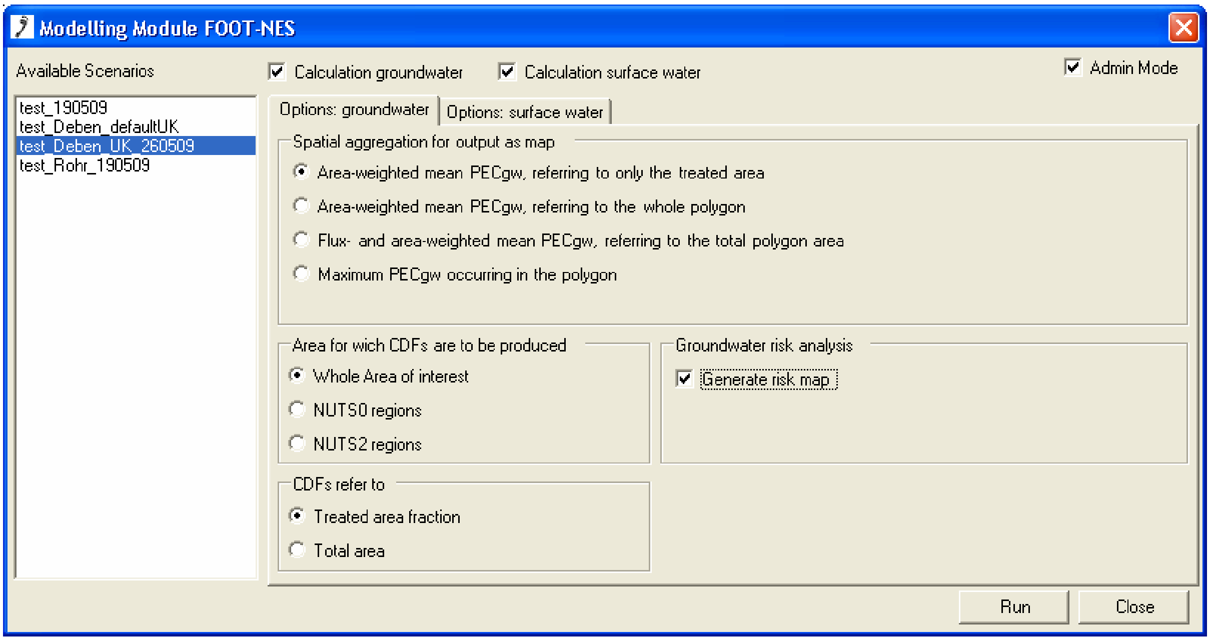


Figure 50 - The FOOT-NES Modelling Module, Tab “Options Groundwater”

Tab “Options surface water”

Apart from the group boxes with options for spatial aggregation, this tab has two other group boxes (Fig. 51):

- In the group box “Output” the user specifies the desired output variables:
  - Pesticide edge-of-field losses (surface runoff, erosion, drainage, lateral subsurface flow)
  - Pesticide inputs into surface waters (surface, runoff, erosion, drainage, lateral subsurface flow, drift)
  - Predicted Environmental Concentrations (PEC) in surface water and sediment (for i) drift, ii) drainage, iii) surface runoff + erosion + lateral subsurface flow)
  - Time Weighted Average Concentrations (TWAC) in surface water and sediment (for i) drift, ii) drainage, iii) surface runoff + erosion + lateral subsurface flow)
- In the group box “Surface water body type” the user selects the water body type into which pesticide inputs are simulated: ditch, stream or pond (cf. section 5.4.1 of chapter 3).

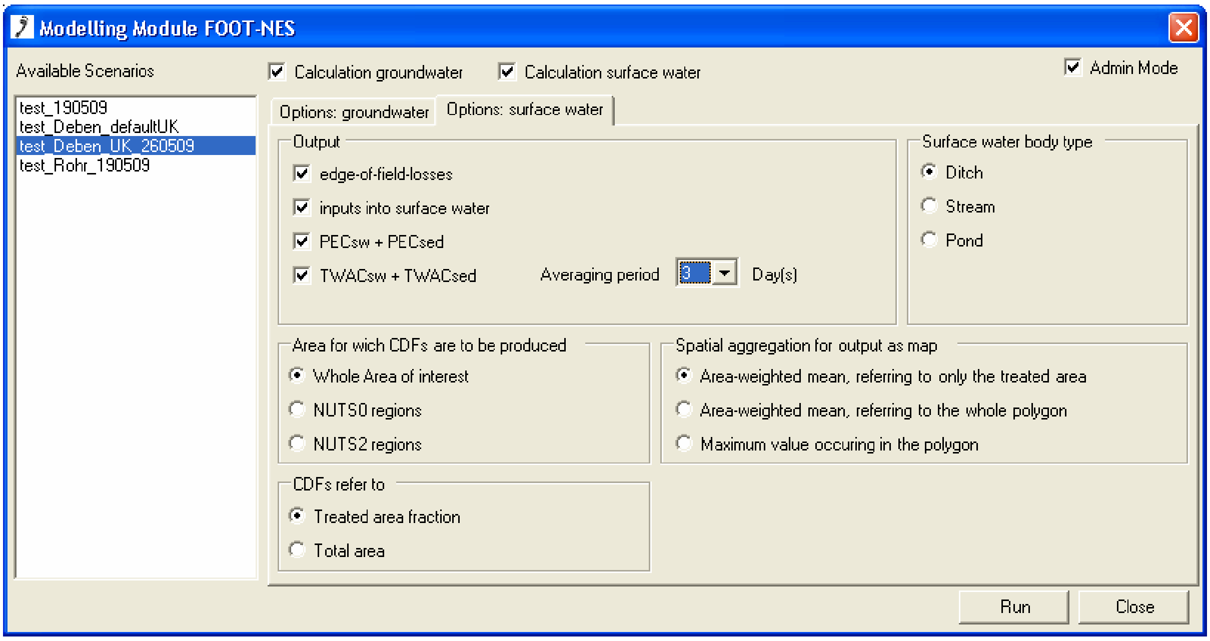


Figure 51 - The FOOT-NES Modelling Module, Tab "Options Surface water"

Running the Modelling Module

After setting all options in the desired way, the user can launch the Modelling Module by clicking on "Run".

The Modelling Module produces

- an output shapefile with the selected output variables as columns in the attribute table
- spatial cumulative distribution functions (CDFs) for the selected output variables as .dbf tables.
- Basic spatial CDF graphs (Fig. 52) based on the .dbf files mentioned above. These graphs can be accessed in ArcGIS under Tools/Graphs and be saved in different graphics formats. Note that these graphs are only temporary and are lost when closing ArcGIS, unless they have been saved by the user by simply saving the current ArcMap Document (.mxd).
- for each run, a small .txt file that documents the pesticide application scenario used and the options selected.

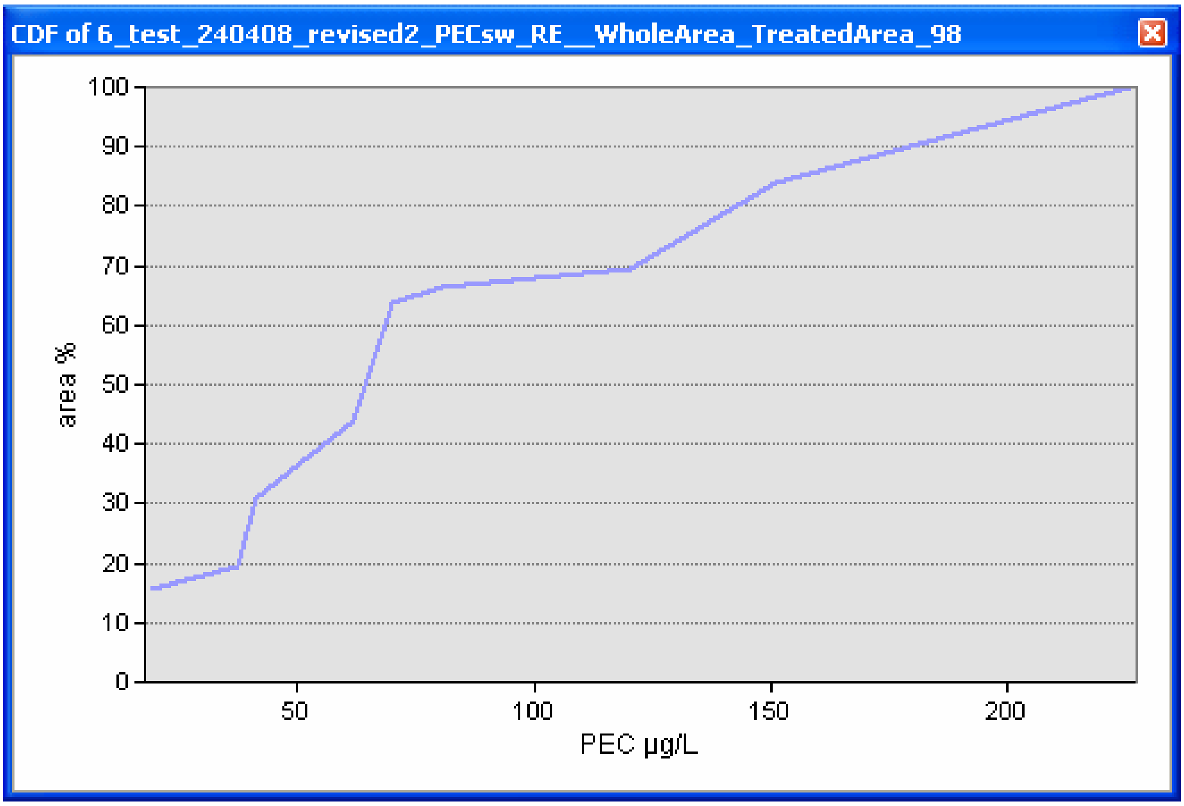


Figure 52 - The FOOT-NES Modelling Module, example graph of a spatial CDF

3.2.8 The FOOT-NES Communication and Reporting Module

Apart from presenting the results of the Dominant Pathways Module, the task of the Communication and Reporting Module is to display the output variables produced by the Modelling Module (maps and CDFs). To enable the display of results, the user first has to select in ArcGIS an output shapefile produced by the modelling module (Fig. 53).

Tab "Map results"

When an output shapefile has been selected, the user can browse through a dedicated tree structure (Fig. 54) to the variable to be displayed as a map. After clicking on the variable, the Communication and Reporting module automatically creates a standard legend in ArcGIS (cf. Fig. 53). Of course, the user can change this legend manually in ArcGIS.

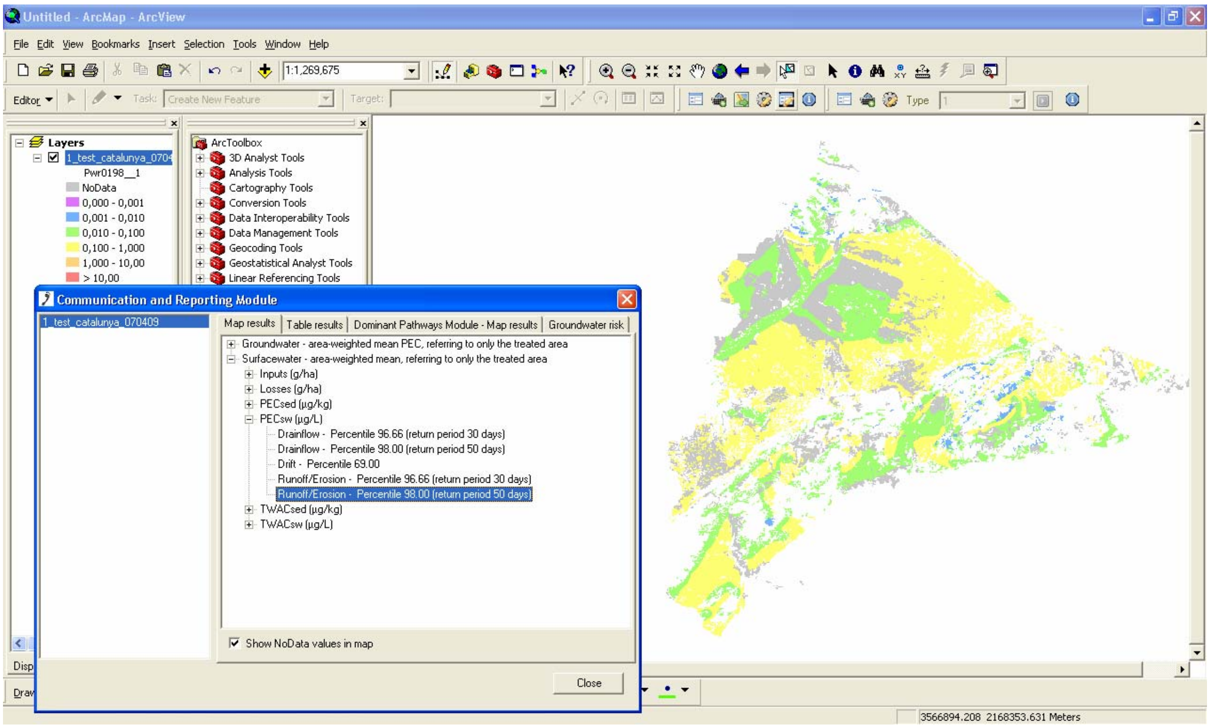


Figure 53 - ArcGIS screen with a FOOT-NES results shapefile and the FOOT-NES Communication and Reporting module, Tab “Map results”

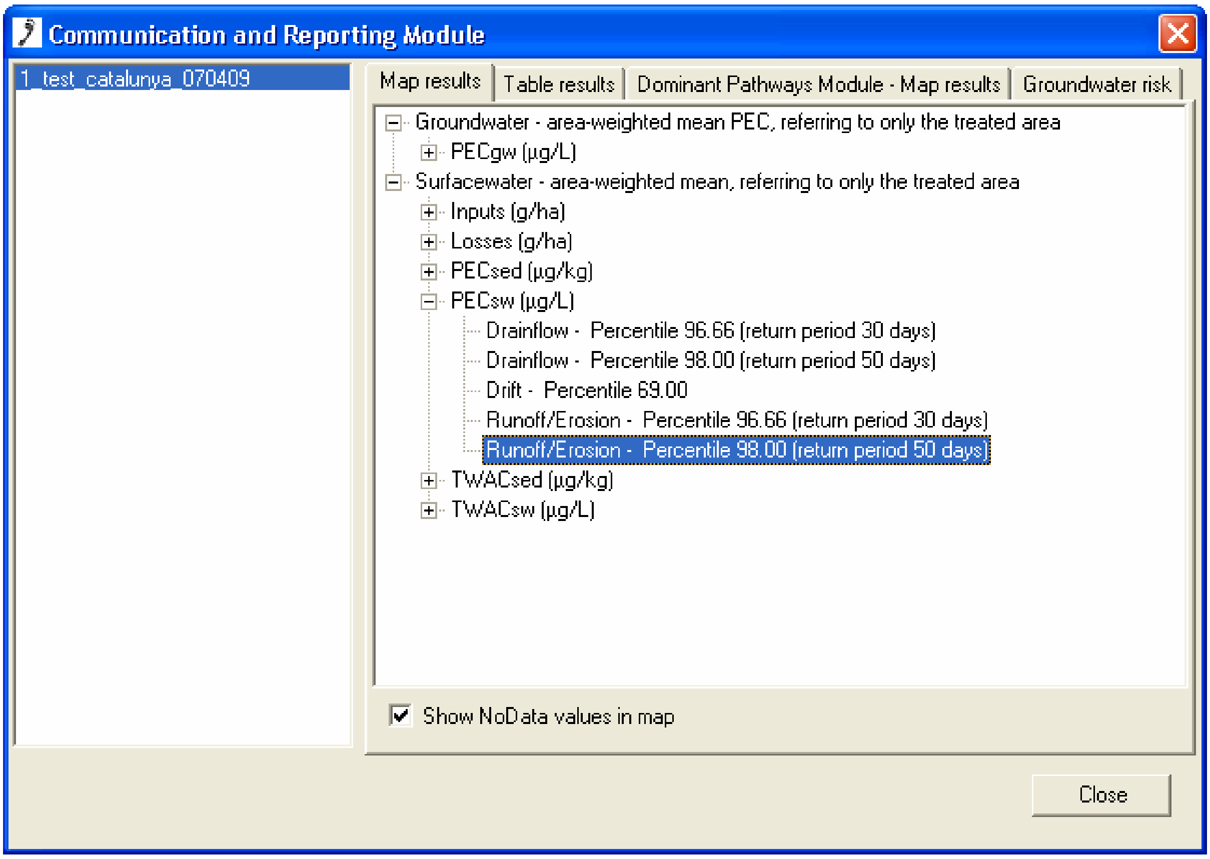


Figure 54 - The FOOT-NES Communication and Reporting module, Tab “Map results”

Tab "Table results"

In this tab (Fig. 55), the user can the user can browse through an identical tree structure as in the "Map results" tab to the variable for which the spatial Cumulative Distribution Functions (CDF) shall be examined. After clicking on the variable, the Communication and Reporting module accesses the corresponding .dbf file produced by the Modelling Module, which contains the spatial CDF of the output variable of concern.

There are two group boxes on the "Table results" tab:

- In the group box "Display percentiles" several standard percentiles and one user-defined percentiles are automatically calculated and displayed. A facility for exporting the calculated percentiles in txt format is still under construction, but will be implemented before the public release of FOOT-NES v.1.
- The group box "Display frequencies" works the other way round: The user enters a value (e.g. a given ecotoxicological threshold in case of PECsw), upon which the corresponding cumulative relative frequency and its complement, the area percentage of exceedance, are automatically calculated and displayed.

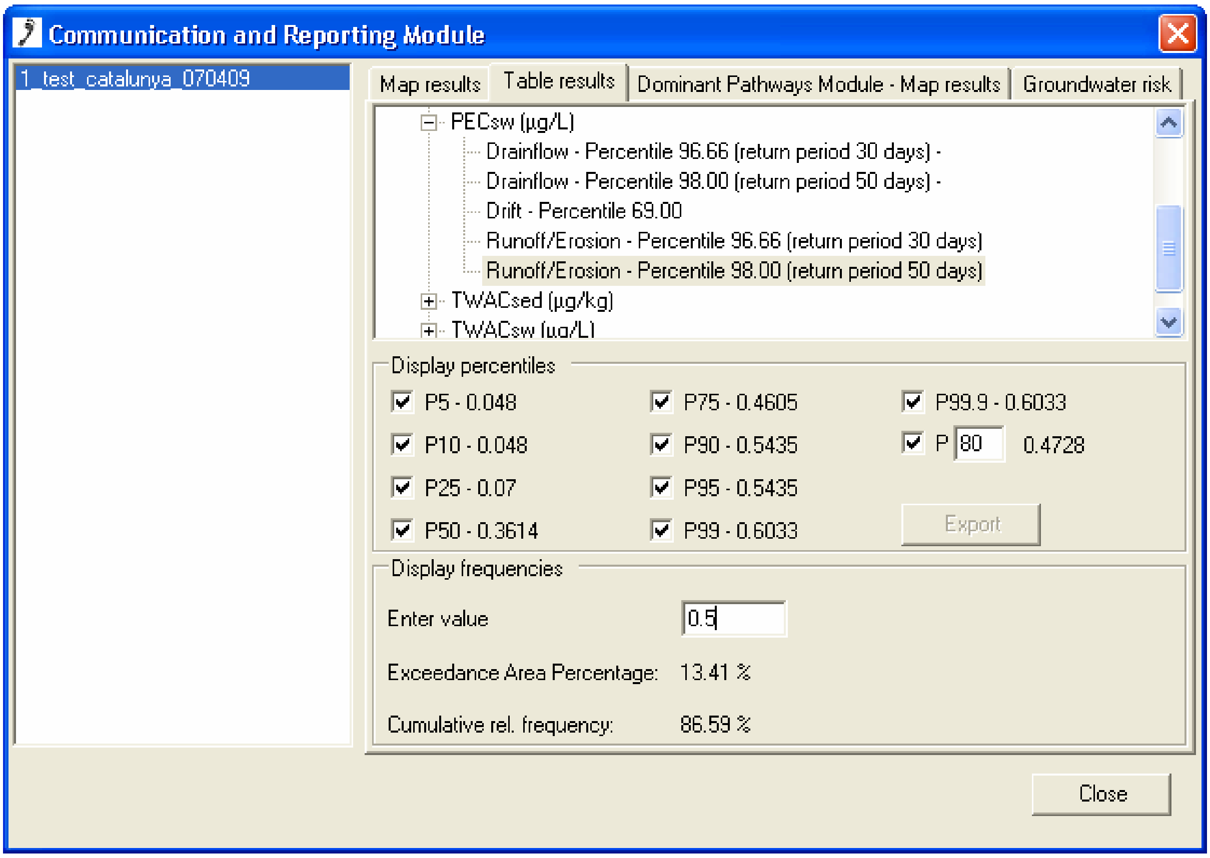


Figure 55 - The FOOT-NES Communication and Reporting module, Tab "Table results"

Tab "Dominant Pathways Module – Map results"

With this tab, the user can view the output of the Dominant Pathways Module (cf. Section 3.2.7). Again, there is a tree structure in place to browse to the desired output variable, and standard legends for the output variables are created (Fig. 56).

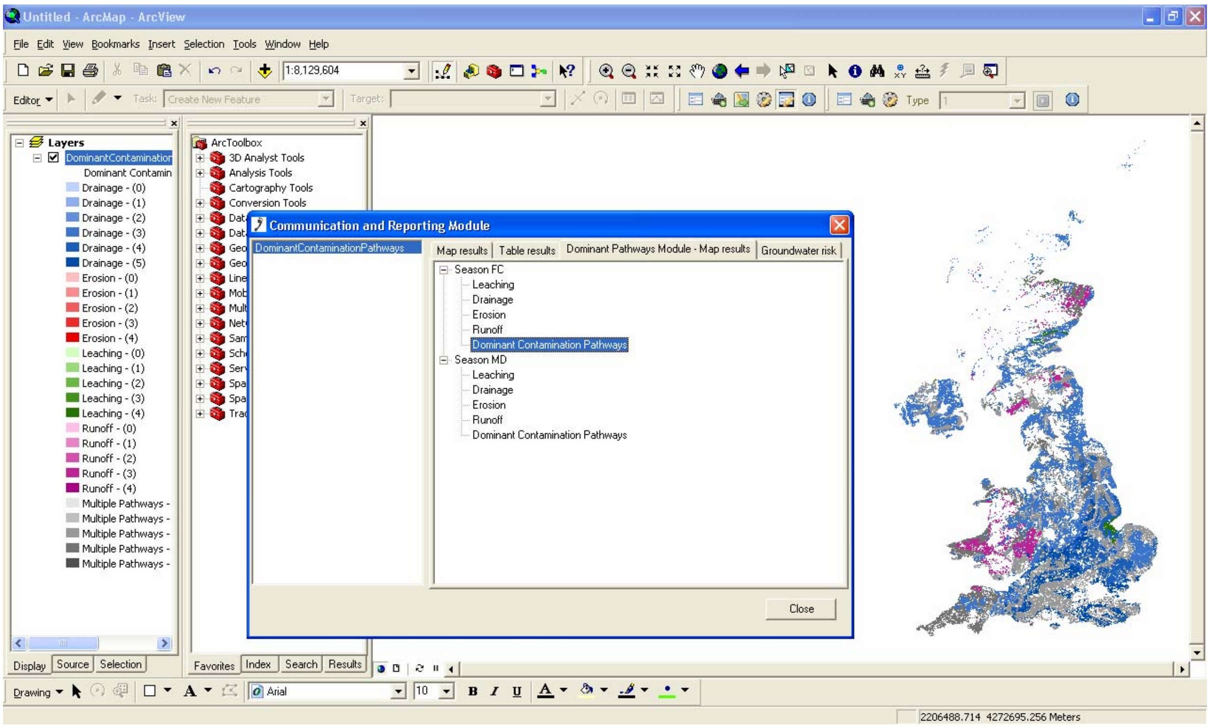


Figure 56 - The FOOT-NES Communication and Reporting module, Tab “Dominant Pathways Module – Map results”

Tab “Groundwater risk”

With this tab, the user can view the colour-coded groundwater risk map (Fig. 57; cf. section 5.3.4 in chapter 3). This map contains two variables in its attribute table:

- Risk class (values from 1 to 5) for soils with PECgw as flux concentration (leaching concentration type 1)
- Risk class (values from 1 to 5) for soils with PECgw as resident concentration (leaching concentration type 2)

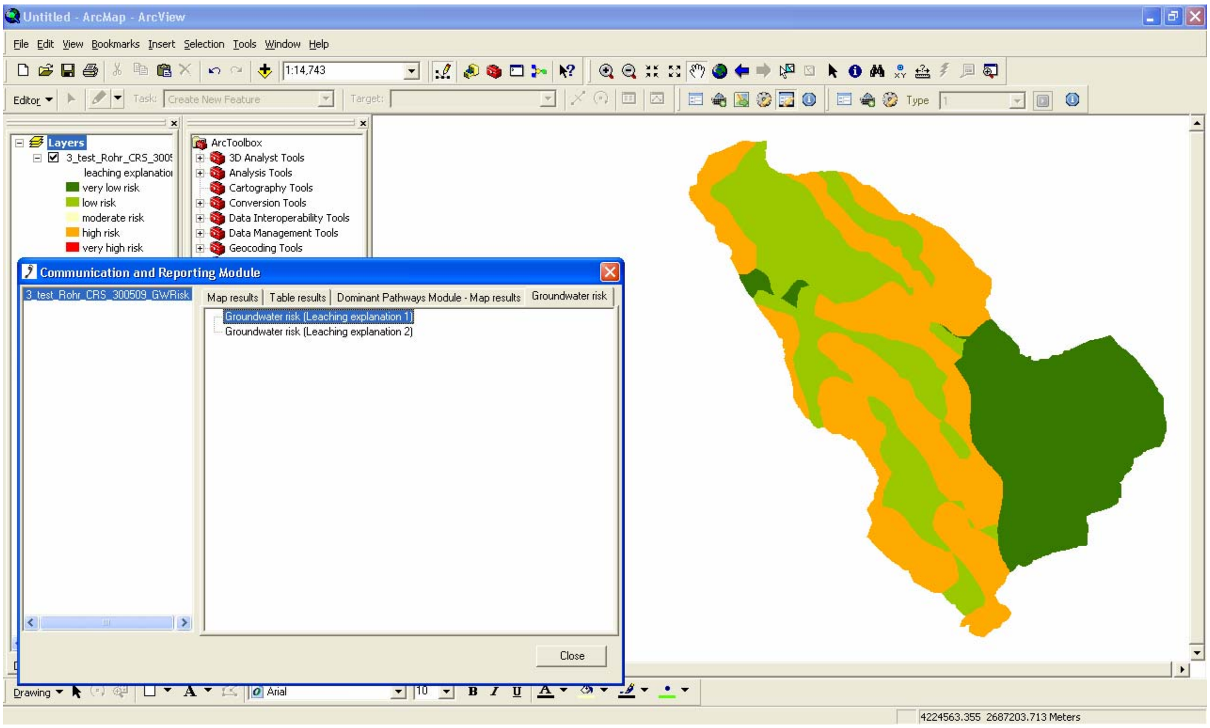


Figure 57 -The FOOT-NES Communication and Reporting module, Tab "Groundwater risk"

4 THE FOOTPRINT PPDB

4.1 Introduction

4.1.1 What is the FOOTPRINT PPDB

The FOOTPRINT PPDB is the Pesticide Properties Database that is utilised by all the FOOTPRINT tools as a source of active substances and their properties. The database is described in detail in Deliverable DL24 (Lewis et al., 2007), but a summary is also provided here. The FOOTPRINT PPDB is a sub-set of the full PPDB managed and maintained by the Agriculture and Environment Research Unit (AERU) at the University of Hertfordshire, UK.

The objectives of the PPDB are to provide:

- A single, comprehensive resource of reliable, consistently presented pesticide data
- A portable format for direct linking to software applications
- Simple online access supported by layperson interpretations and user tools

The PPDB currently holds ~1000 records for active ingredients, plus 480 records for metabolites. The data include general information, physicochemical and environmental fate data, acute and chronic endpoints for a range of fauna and flora and information on human health issues.

4.1.2 Background

The origins of the full PPDB can be traced back to 1994 to the development of the award winning Environmental Management for Agriculture (EMA) software (Lewis & Bardon, 1998). The PPDB has been further developed during the FOOTPRINT project (2006-2009) and specific tools and facilities have been developed to meet the needs of the FOOTPRINT project and the FOOTPRINT tools that have been developed. It was also considered beneficial to ensure that the database was also available as an online resource open and free-of-charge to all interested parties, so online facilities have also been developed during this time.

4.2 Data management

4.2.1 Review of existing resources

Before construction and population of the FOOTPRINT PPDB began a review of existing resources and their ability to fulfil the needs of both the FOOTPRINT project and those of other users of pesticide fate and ecotoxicological data was undertaken. The study concluded that existing resources fell short of the ideal both with respect to the number of pesticides that were included and the range of parameters available. In addition the review identified problems associated with format, updating, maintenance and language barriers.

4.2.2 Maintenance

Data are maintained regularly and the range of pesticides and data held is under constant review based on demand. Data has been cross-checked against a number of other resources and agreements to share data with holders of other databases have been put in place.

A PPDB management tool has also been developed that ensures the structural integrity of the database is maintained and which simplifies the process of updating existing records and adding new records. It also provides a facility to export sub-sets of data into different formats (e.g. differently structured MS Access databases, Excel spreadsheets and CSV files). This allows us to provide the database in a format that suits the needs of a range of different end users, including the three FOOT tools.

4.2.3 Fitness for purpose

Risk assessment procedures rely heavily on the accuracy of the data used to drive them. Data quality and 'fitness for purpose' have been handled with in the PPDB by assigning each parameter with a confidence code that reflects the data source and the confidence data administrators have in the value.

4.3 Use of the FOOTPRINT PPDB

4.3.1 To support the three FOOT-Tools

Each of the FOOT tools (FS, CRS and NES) requires a version of the FOOTPRINT PPDB. They use the FOOTPRINT PPDB in two ways. Firstly to populate a list of active substances for the user to select when building their pesticide programme and, secondly, as a source for the fate and ecotoxicity property values. In order to satisfy the requirements of each tool the FOOTPRINT PPDB is exported from the full PPDB in slightly different structures using the PPDB management tool described above. The structural requirements of each tool are stored in a schema file that can be loaded each time a new FOOTPRINT PPDB needs to be created.

In the case of FOOT-FS, updates to the FOOTPRINT PPDB are uploaded to a web server. Then (as described above) these can be automatically downloaded by FOOT-FS to update the database used within the software when making calculations.

4.3.2 FOOTPRINT PPDB online

As described above, one of the objectives was to provide simple online access to the PPDB so that anyone around the world can access the data held within the PPDB. To achieve this objective a tool was developed to extract the data from the MS Access database and create static html pages. These pages are then delivered through a number of different web portals including:

- The FOOTPRINT web site – http://www.eu-footprint.org/ppdb.html
- The PPDB page – http://www.herts.ac.uk/aeru/footprint
- IUPAC - http://agrochemicals.iupac.org/
- ADLib - http://www.adlib.ac.uk/

The online FOOTPRINT PPDB is currently available in 6 languages: English, French, Italian, Polish, Slovenian and Spanish.

Statistical monitoring of the online database usage is undertaken. As of May 2009, the FOOTPRINT PPDB receives on average ~2000 hits per day from ~800 users around the world. The figures continue to increase each month.

5 DISCUSSION AND PERSPECTIVES

In chapter 4, the latest versions of the three FOOT tools were presented. The final versions (v. 1.0) of three FOOT tools are expected to be released to the public on the FOOTPRINT website in early 2010. Default data sets, user support (user manual, help section, videos) and documentation (technical report) will be produced along with the tools.

Any software must be maintained and regularly updated to ensure its continuing use in the future. Support must be provided to those users that encounter problems which cannot be fixed by consulting the User Manual or the Help Section. It is proposed that the start-up company FOOTWAYS which was created on 1 June 2009 by the former FOOTPRINT coordinator acts as the official FOOTPRINT dissemination body, which would provide long-term support for the FOOTPRINT tools. This would have to be endorsed by FOOTPRINT partners through the signature of a Use and Dissemination Agreement.

As regards regular updates, there are already ideas for further improvements of the FOOT tools. For instance, it turned out that MS Access is not particularly suited for dealing with large amounts of data: it is slow, does not fully support SQL standards and has a maximum file size of 2 GB. These shortcomings are less of a problem with FOOT-FS, where the amounts of data handled at the same time are relatively small. However, they are a major issue for the two GIS based tools FOOT-NES and especially FOOT-CRS. For these reasons, one of the possible developments is to switch from MS Access to a free, open-source database software, e.g. PostgreSQL or SQLite, in the next major update (v. 2.0) of FOOT-CRS and FOOT-NES. The release of this update is envisaged for late 2010 or 2011.

CHAPTER 5 – EVALUATION OF THE SPATIAL TOOLS

The purpose of this activity is to evaluate both the reliability and usability of the FOOT-CRS and FOOT-NES tool. The objectives were to first beta test each tool prototype for bugs and operational efficiency, followed by evaluation of the operational tool using datasets collected from different climatic, geological and agricultural regions within Europe. However, as a full set of modelling results from Work Package 4 were not available in time for completion of this report, it has not been possible to compare the modelling results produced by the tool with the available monitoring datasets. Instead full beta testing of the FOOT-NES tool has been carried out and its utility and performance evaluated using a set of 'dummy results' comprising synthetic modeling results for each country or region. Unfortunately, because of the resignation of GEOSYS, the Consortium Partner responsible for development of FOOT-CRS, a fully functional beta version of the tool has not been available for comprehensive testing. As a result only limited evaluation of the FOOT-CRS utility has been possible

1 EVALUATION OF FOOT-CRS

In the following section, the areas and data available for evaluation of the FOOT-CRS tool are described followed by an overview of the tool's current functionality based on the work of one FOOTPRINT partner (University of Giessen).

1.1 Evaluation sites selected

The FOOT-CRS tool was evaluated in 14 catchment areas representing different climatic, geological and agricultural regions within Europe. The main characteristics of the various sites is summarised in Table 23, while the catchment locations and detailed site descriptions are given in DL38 (Kjær *et al.,* 2009).

	Size (km2)	Elevation (m a.s.l.)	Mean precip. (mm/y)	% agricultural land	Dominating crop type
Switzerland					
Rohr	2	490-550	1330	89%	[21]
Greifensee	167	435-1100[1]	1330	54%	[21]
Murtensee	693	429-1512[1]	846	69%	[21]
The Swiss Rhine basin	28055	246-4274[1]	1166	51%	[21]
Slovenia					
The Apace Valley	44	220	916	69%	Cereals (80%) Rape (14%) Root crops (5%)
France					
Bruyères-et-Montbérault	2	150-200	695	80%	Cereals (55%) Sugar beet (20%) Peas (6-20%)
Ouarville	18	148-155	605	83%	Cereals (56%) Rape (14%) Peas (10%)
Poland					
Ciesielska Woda	33	147 – 213	520	87%	Cereals (75%) Potatoes (75%) Rape (7%)
England					
Deben	176	0 – 68	575	94%	Cereals (49%) Rape (9%) Sugar beet (5%)
Upper Cherwell	206	91 – 224	650	82%	Cereals (30%) Grass (32%) Rape (8%)
Leam	369	49 – 215	650	77%	Cereals (28%) Grass (32%) Rape (6%)
Teme	1652	12 – 540[1]	800	74%	Grass (48%) Cereals (16%) Rape (2%)
Wensum	557	0 – 108	670	72%	Cereals (32%) Grass (12%) Rape (4%)
East Anglia: Little Ouse, Wissey & Lark	4200	-8 – 131	600	76%	Cereals (36%) Sugar beet (8%) Rape (4%) Potatoes (3%)

Mean Precip: mean annual precipitation (mm/y). [1] *Most agricultural land is below 1000 m (Greifensee, Murtensee and Swiss Rhine basin) and 300 m (Teme).* [2] *Data not yet available*

Table 23 -Characteristics of the sites included in the evaluation if the CRS tool

1.2 Data available for evaluation

Each partner assembled two sets of data to carry out the evaluation of FOOT-NES in their area.

1.2.1 Data available to create detailed agro-environmental scenarios

Within the FOOTPRINT tool a set of European-level ‘default’ data files providing a full parameterisation of the required environmental characteristics of a given area is available to the user. However, the users can also create their own agro-environmental scenarios (using the Data Management Module) based on their own, more detailed soil, land use/land cover and cropping data. At present it is not possible to incorporate more detailed climate data into the scenarios. As part of the evaluation process such detailed agro-environmental scenarios were established based on the local data collected from each of the 14 sites. Detailed local data on land cover and crop distribution were collected from all evaluation sites. Moreover all sites had a detailed soil map available allowing a more detailed parameterisation of the soils using the FOOTPRINT soil selector. Additional description of the available data is given in DL38 (Kjær *et al.*, 2009).

1.2.2 Data available to evaluate the FOOT-CRS modelling results

Comprehensive datasets describing both pesticide usage and monitoring results in groundwater and surface water bodies were established for all sites. In total the collected monitoring dataset comprised 150 pesticide-site combinations. Data on pesticide usage, e.g. date of application, application rate as well as area of treated crop was assessed from either field survey or local agricultural statistics made available to each partner. The collected data are briefly summarised in Tables 24 and 25. and further detailed in DL38 (Kjær *et al.*, 2009). The monitoring data from Ciesielska Woda (Poland) are very limited (cf. Table 24 and 25). In the Ciesielska Woda catchment FOOT-CRS will thus be evaluated by comparing output from the FOOT-CRS tool with the groundwater vulnerability map obtained with the Attenuation Factor approach (Rao *et al.*, 1985).

	Apace Valley (Slovenia)	Bruyères-et-Montbérault (France)	Ouarville (France)	Ciesielska Woda (Poland)	East Anglia groundwater (England)
Groundwater monitoring					
Number of samples	1192	792	3312	2	337
No. of pesticides	6	41	11	33	8
No. of sampling points	15	14	10	1	20
Sampling frequency (times/per year)	12	4	12	2	1 - 2
Monitoring period	1993-2000; 2006-2008	1998-1999	1999-2004	2008	2006-2008
Available pesticide usage data	1992-2001; 2006-2008	1989-1997	1997-2003	2002-2005	2006 - 2008

Table 24 -Overview of the groundwater monitoring and pesticide usage data collected for evaluating the CRS tool.

	Rohr (CH[1])	Greifensee (CH[1])	Murtensee (CH[1])	Swiss Rhine Basin (CH[1])	Apace Valley (Slovenia)	Ciesielska Woda (Poland)	Deben (England)	Upper Cherwell (England)	Leam (England)	Teme (England)	Wensum (England)
Surface water monitoring											
No. of samples	600			3651	494	4	224	1522	2836	764	987
No. of pesticides	3	1	1	1	6	33	9	7	6	9	9
No of sampling points	3 2)	1 3)	1 3)	1	7	2	5	1	1	2	3
Sampling frequency (times/per year)				365	12	2	12	25-102	29-70	16-60	16
Monitoring period (years)	2000 2)	1990-2002 4)	1997-2003	1995-2004	1993-2000 2006-2008	2008	2007	2001-2006	2001-2006	2006-2008	2006-2008
Available pesticide usage data	2000	1990-2002[4)]	1997-2003	1995-2004	1992-2001 2006-2008	2002-2005	2007	2001-2006	2001-2006	2006-2008	2006-2008

[1)] *Switzerland.*
[2)] *Flow proportional sampling of high temporal resolution was carried out during April – August 2000.*
[3)] *River concentrations have been back-calculated by inverse modelling from measured lake concentrations.*
[4)] *No monitoring was conducted in 1992, 1995 and 1996.*

Table 25 -Overview of the surface water monitoring and pesticide usage data collected for evaluating the CRS tool.

1.3 Utility of the FOOT-CRS tool

FOOT-CRS includes five modules: the *Pesticide Scenario Manager*, the *Data Management Module*, the *Dominant Pathways Module*, the *Modelling Module* and the *Communication and Reporting Module*. However, only the Pesticide Scenario Manager and the Data Management module are fully functional at the moment and only one Partner was able to undertake any sort of evaluation of the current utility of the tool using the version 0.5.3417.38087 (note that the latest version 0.7.12 is substantially more advanced and bug-fixed than the version tested).

Neither the Dominant Pathways module nor the Communication and Reporting module are yet available for evaluation but, as these modules will be very similar to those of FOOT-NES, which are currently operating well, no problems are anticipated in incorporating these before the end of the project.

The Data Management module is complete and fully functional although some minor improvements are still needed. These relate to the incorporation of messages and warnings for the user and refinement of the re-sampling resolution of the zonal statistics discharge grids in order to create suitable area-specific discharge data for each polygon.

The Pesticide Scenario Manager is fully functional, but has not been evaluated in WP6 because it became available only after the completion of DL38.

The Modelling module is only partially complete. Groundwater calculations and calculation of drainage losses, inputs and PECsw are working, as is the grid-based runoff routing procedure and the calculation of pesticide inputs into surface water via surface runoff and erosion. However, the calculation of PECsw due to surface runoff and drainage inputs is not operational yet.

In summary, although there has been substantial progress in the development of the FOOT-CRS software since the FOOTPRINT Final Conference in March 2009, the version available now is not yet a fully functional beta-version.

1.4 Perspectives

Beta testing of the FOOT-CRS tool is at an intermediate stage and although many problems have been identified and corrected, some problems still remain and the testing process clearly has to continue until the final version is available. The latest version of the tool at the time of writing this report is 0.7.12 (dated 19 January 2010). Nevertheless, the limited evaluation carried out has shown that the tool will be complex and probably require a good technical knowledge of ArcGIS techniques to operate efficiently. As with the FOOT-NES tool, users will also need a clear understanding of the different datasets that are required by the tool, and the necessary format of folder and data file names. In particular, it is important to ensure that the file and folder names specified in the Data Management module are in a format compatible with Arc-GIS, with no blank spaces in the names.

In order to carry out a proper evaluation of the reliability of FOOT-CRS, five partners have assembled a comprehensive set of catchment level pesticide usage and monitoring data, as well as detailed environmental information on the distribution of local soil types, land cover and crops. This information covers 11 surface water catchments with sizes ranging from 2 km^2 to 28055 km^2 and 5 groundwater catchments with sizes range from 2 km^2 to 4200 km^2. It includes a range of different climatic, geological and agricultural regions within Europe and provides an excellent set of data for evaluating the validity of the tool predictions.

In summary, the FOOT-CRS tool is still under development and requires further comprehensive beta testing before it can be considered fully functional. For the future, it is recommended that:

- A full beta testing schedule is developed with the current partners to test the tool's operation in different countries, crops and climates and to quantify the modelling running times for both the default and user-defined detailed agro-environmental scenarios in each of the characterized catchments.
- A clear step-by-step User Manual is written to guide users through installation and operation of the tool.
- Internal error checking and associated warning messages are built into the tool to ensure that file and folder names have the correct format.
- Further work is carried out to improve the 'help' routines associated with each module, especially explanation of the different types of results data that are specified in the Pesticide Scenario manager and Modelling Modules and presented in the Communication & Reporting Module.

- A full evaluation of the tool model predictions against monitoring data results is carried out for all the characterized catchments once the FOOT-CRS tool is fully functional and the FOOTPRINT modelling databases are complete.

2 EVALUATION OF FOOT- NES

In this section, the areas and data available for evaluation of the FOOT-NES tool are described followed by an assessment of the utility of each of the FOOT-NES tool modules.

2.1 Evaluation sites selected

THE FOOT-NES tool was evaluated in five areas representing different climatic, geological and agricultural regions within Europe. These five areas represent a range of different climatic, geological and agricultural regions within Europe. The location and main characteristics of the various sites is summarised in Figure 58 and Table 26, whereas detailed site descriptions are given in DL39 (Hollis et al., 2009).

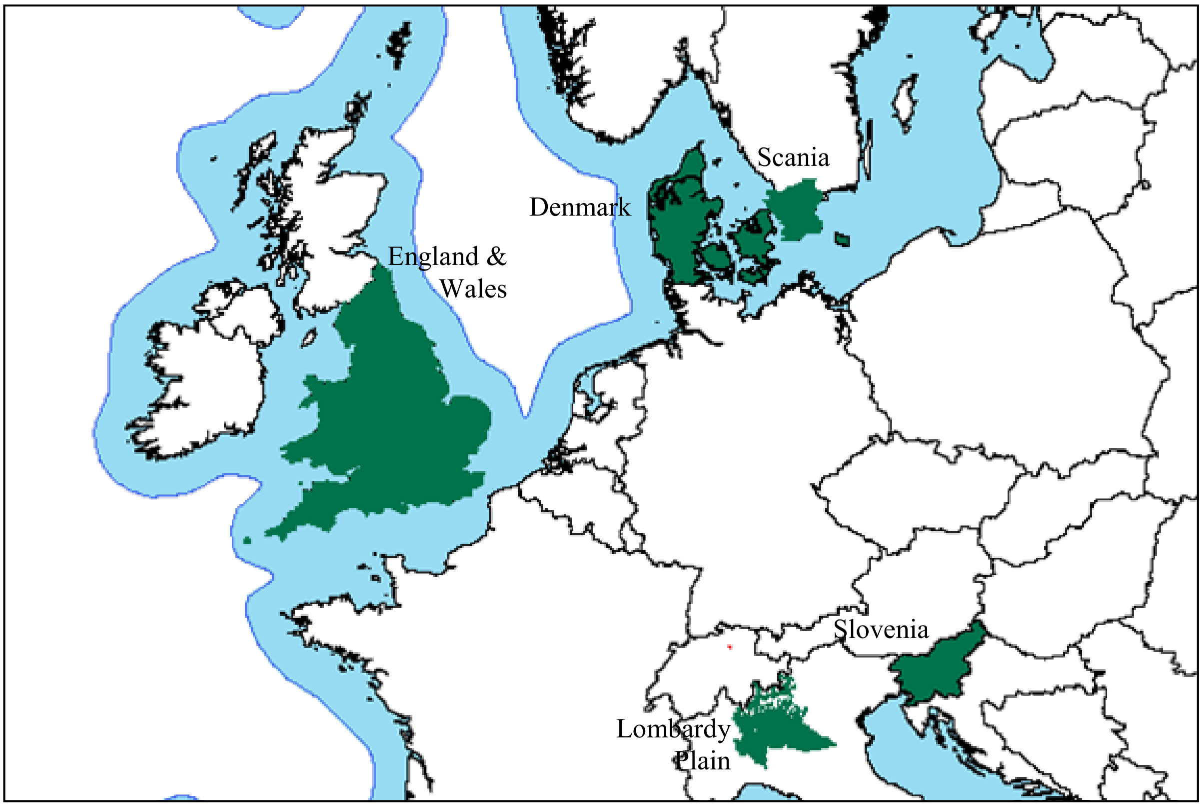


Figure 58 - Location of test regions used to evaluate FOOT-NES

	Scania (Sweden)	The Lombardy Plain (Italy)	Denmark	England & Wales	Slovenia
Size (km^2)	11,346	13,500	43,094	151,010	20,273
Elevation (m a.s.l.)	0-212	8-1150 [1]	0-170	0 – 1000 [1]	0 – 2864 [1]
Mean precip. (mm/y)	700	858	712	700	1250
Mean E_{pot} (mm/y)	760	755	582	550	600
% agricultural land	41%	85%	60%	60%	20%
Dominating crop type	Cereals	Maize & Rice	Cereals	Cereals	Wheat, Maize & Potatoes
D.C.P.	Drainage and leaching [2]	Drainage and leaching	Drainage and leaching	Drainage and leaching [2]	Drainage and leaching

E_{pot}: Potential evapotranspiration; D.C.P.: dominating contamination pathways
[1] Most agricultural land is below 600 m (England) 100 m (Lombardy) and 600 m (Slovenia);
[2] Surface runoff/erosion undoubtedly occurs commonly within fields, but very little data is available to indicate how much and how frequently such runoff reaches surface water bodies.

Table 26 -Overall characteristics of the sites included in the evaluation of the FOOT-NES tool

2.2 Data available for evaluation

Each partner assembled two sets of data to carry out the evaluation of FOOT-NES in their Area.

2.2.1 Data available to create Regionally-specific detailed agro-environmental scenarios

Within the FOOTPRINT tool a set of European-level default data files providing a full parameterisation of the required environmental characteristics of a given area is available for the user. However, the user can also create their own agro-environmental scenarios (using the Data Management Module) based on their own, more detailed soil, land cover, cropping and discharge data. At present it is not possible to incorporate more detailed climate data into the scenarios.

As part of the evaluation process such detailed agro-environmental scenarios were established based on the local data collected from each of the five sites. While land cover was based on default data being available within the FOOTPRINT project, detailed data on crop distribution within each municipality (Scania, Lombardy & Slovenia), 1 × 1 km^2 grid (Denmark), or 5 × 5 km^2 grid (England & Wales) was collected from each of the evaluation sites. Moreover all sites had a detailed soil map available with a higher spatial resolution than the EU-level default soil map (1:1000000). The local soil types were translated into FOOTPRINT soil types with the FOOTPRINT soil selector. Additional description of the available data is given in DL39 (Hollis et al., 2009).

2.2.2 Data available to evaluate the FOOT-NES modelling results

Comprehensive datasets describing both pesticide usage and monitoring results in ground and surface water bodies were established for all sites. In total the collected monitoring dataset comprises 70 pesticide-site combinations. Data on pesticide usage e.g. application rate and area of treated crop were assessed from national or regional statistics made available to each partner. Where possible, these statistics were also used to derive the date of application but in some cases this date was derived by expert judgement. The collected data are briefly summarised in Table 27 and further detailed in Hollis et al. (2009).

	Scania (Sweden)	The Lombardy Plain (Italy)	Denmark	England & Wales	Slovenia
Groundwater monitoring					
No. of samples	526	1612	5,115	12,072	526
No. of pesticides	4	4	14	7	6
No. of sampling points	416	460	845	3,503	18
Sampling frequency (times/per year)	Not known	2	1	1-2	12
Monitoring period (years)	4	3	16	8	6
Surface water monitoring					
No. of samples	534	1733	321	24,600	*
No. of pesticides	4	4	14	7	*
No. of sampling points	34	154	7	590	*
Sampling frequency (times/per year)	Not known	Occasional	12	4-12	*
Monitoring period (years)	4	3	7	8	*
Available pesticide usage data					
National statistics	1999-2003	2007	1989-2007	1990-2007	2003-2008

* monitoring data for surface waters not evaluated

Table 27 -Overview of pesticide data collected for evaluating the NES tool

2.3 Utility of the tools

FOOT-NES includes five modules: The *Pesticide Scenario Manager*, the *Data Management Module*, the *Dominant Pathways Module*, the *Modelling Module* and the *Communication and Reporting Module*. Their utility was tested in various versions between January & May 2009. Identified bugs were regularly reported during this beta testing phase, resulting in frequent updates of the tool. The last version tested, which worked on all the machines and scenarios used, was version 0.5.3406.31532 (note that the latest version is 0.7.12). The specifications of the machines used to evaluate the FOOT-NES tool varied from moderate to high. This information is summarized in Table 28.

	Machine type	Processor	RAM	Hard Disk Capacity
Scania	High spec	Intel Core Duo, 2.66 GHz	3.23 GB	1 x 148 GB
Lombardy Plain	High spec	Intel Pentium M760, 2 GHz	1 GB/Go	1 x 160 GB
Denmark	High spec	Intel Core Duo, 2.2 GHz,	4.00 GB	1 x 96 GB
England & Wales	High spec Moderate spec	Intel Xeon, 2.5 GHz Intel Celeron, 1.5 GHz	3.25 GB 448 MB	2 x 500 GB 1 x 55.8 GB
Slovenia	High spec	Intel Core Duo, 2.33 GHz	1.98 GB	1 x 300 GB

Table 28 -Specifications of the machines used for beta testing of FOOT-NES

2.3.1 The Data Management Module

The Data Management Module has two functions: Firstly to ensure that all the 'environmental' input data required by the models are available and placed in specified locations. Secondly to enable the user to create their own agro-environmental scenarios based on their own, more detailed soil, land cover, cropping and/or discharge data. At present it is not possible to incorporate more detailed climate data into the scenarios. Before any modelling runs can be carried out using the Modelling Module or contaminant pathways mapped using the Dominant Pathways Module, the Data Management Module must be used to define projects. However, there is an important distinction between using the Module to define projects utilizing the FOOTPRINT 'Default Data sets' and those utilizing the user's own more detailed data sets.

Using the FOOTPRINT Default Data: Using the module to set up a project based on the FOOTPRINT default data is very straightforward. The only things necessary are to specify the location of the FOOT-NES working directory and the folder in which the default data is stored (this is done using the 'Project' tab) and then to specify the location of the different FOOTPRINT default data files needed (this is done using the 'General' tab). No other tabs in the module should be used and the project is then simply saved by naming it in the appropriate box under the ‘Project’ tab and using the ‘Save’ button at the base of the module window. It is important NOT to use the ‘Create’ button for any default projects and it is best to use only one named default project for all modelling and mapping operations based on the FOOTPRINT default data sets.

Using more region-specific data sets to create Detailed agro-environmental scenario projects: Using the module to set up a project based on the user’s more detailed Region-specific datasets is less straightforward as it requires users to complete other tabs in the module covering ‘Land cover/land use map’, ‘Soil map’, ‘Surface water body characteristics’ and ‘Discharge’. Under these tabs, the location of the user’s own data files are specified together with the conversion of their own data codes to those required by FOOTPRINT. For both the ‘Land cover / Land use map’ and the ‘Soil map’, the conversion process can be done manually or, if the user’s codes are already in FOOTPRINT format, automatically. Bringing the land cover, land use or soil codes into FOOTPRINT format to enable an automatic assignment normally requires pre-processing the data using ArcGIS and/or MS Access independently of FOOT-NES and thus necessitates a good technical understanding of ArcGIS and MS Access. It also requires use of the FOOTPRINT Soil Selector software (cf. DL34 (Lewis & Tzilivakis, 2009a) or flow charts (cf. DL8 (Hollis et al., 2006)) to correlate local soil types with the FOOTPRINT Soil Types.

All five partners successfully used the Data Management module to save a default project and use it in the other FOOT-NES modules. Experiences with creating user-specific projects were more variable, depending on user’s technical understanding of ArcGIS. To the date of Deliverable DL39, only two partners managed to create their own detailed agro-environmental scenarios. As a result of partners’ attempts to create user-specific scenarios, a bug in the “Soil map” tab of the Data Management module was identified and fixed in due course. However, it was not possible for the five partners to test a corrected version in time before completion of the testing exercise.

2.3.2 The Pesticide Scenario Manager

The Pesticide Scenario manager is straightforward to use and all the partners successfully used the module to create compound-specific scenarios for their areas of interest. This applied to areas with agro-environmental scenarios based on both the default data and user-specified detailed data (see section 2.3.1 above). However, two issues need to be highlighted for future consideration:

- Firstly, in order to create the scenario, the ‘Spatially variable application’ tab must be completed even if the user intends to apply only one application rate to all the area of interest. This can be confusing for an inexperienced user and it is recommended that the tab be re-named as ‘Application details’.
- Secondly, when using the ‘Spatially variable application’ tab, once the application rate and date have been defined for the selected polygons, it is necessary to complete the box specifying the ‘Percentage treated of crop group area (%)’ at which point both the ‘target crop’ and ‘crop group’ are displayed on the screen. The reason why the user is asked for a treated percentage of the crop group rather than that of the target crop is because the EU level agricultural statistics used to create the land use component of the default agro-environmental scenarios database have coarser categories than the 42 FOOTPRINT crops. For instance, the EU-level agricultural statistics do not separate winter and spring crops, and amalgamate various species of legumes into the group “pulse”. This distinction between target crop and crop group may also be confusing to inexperienced users. Although there is some brief help text given for this box, it is recommended that such text is expanded to clarify that the selected percentage needs to take into consideration both the estimated percentage of the target crop to which the pesticide of interest is applied within the specified month AND the percentage of the crop group (used in the FOOTPRINT agro-environmental scenarios) that is occupied by the target crop.

In addressing this second issue, most partners used either regional or national statistics on pesticide usage to determine an application rate for the compound of interest, expert judgement to determine a date of application for the compound of interest and then a combination of expert judgement and regional or national cropping statistics to determine the ‘percentage treated crop group area’.

The process of linking these determined data to specific polygons is then completed as follows: First the user selects the mitigation measures they wish to apply (if any) in the tab ‘Spatially variable mitigation measures’. Then, if the user wants to apply the same application scheme to the whole Area Of Interest (AOI) shape file (this is either an agro-environmental scenario shape file or a subset of it), they open the tab ‘Spatially variable application’, press the ‘Define’ tab (which opens the window ‘Spatially variable application and mitigation for selected crop’) and use ArcGIS to select a set of polygons in the AOI. They then define the application rate, application date, percentage treated and final mitigation factors using the relevant tabs and, by pressing the ‘Set’ button, assign the data to the selected polygons. If the user wants to apply different application and/or mitigation criteria to different parts of the

AOI, they must go through the same process for each sub-set of polygons to which they wish to assign specific criteria (cf. section 3.2.5 of chapter 4).

Running times for setting the mitigation and/or application scenarios are good, ranging from a few seconds for small areas comprising between 4 and 15 polygons, to a few minutes for large areas comprising hundreds of polygons. Performance does not seem to be affected by the specification of the machine.

Most partners did not apply any mitigation options when defining their pesticide scenarios because their objective was to create relevant scenarios that could be used to drive the modelling module so that model results (when they become available) could be compared with the available monitoring data. Nevertheless one partner created a specific mitigation scenario in order to confirm that mitigation routines built into the modelling module worked and that model runs using this scenario gave input loads and PECs that were smaller than those for a similar scenario with no mitigation.

2.3.3 The Dominant Pathways Module

All partners found this module straightforward to use, especially as it does not depend on results from the Modelling Module to operate. It also runs quickly: Using the High Specification machine, a run for the whole of the UK (179,000 km^2, 18,189 polygons in the output map) took approximately 90 seconds, whereas on the Moderate Specification machine, a run for the same area took approximately 3 minutes.

However, two points of clarification are needed. Firstly, users need to be aware that, because the output of the Dominant Pathways module is pesticide substance-independent, it works from the currently active agro-environmental scenario (shape file and database) specified in the Data Management module and not the pesticide application scenarios specified the Pesticide Scenario manager. Secondly, users need to be aware that once a module run has completed, mapped results do automatically appear in the ArcGIS main screen, but should be viewed using the Communication and Reporting Module.

2.3.4 The Modelling Module

All partners found the Modelling Module easy to operate. It is not necessary for any shape files or layers to be open for the module to operate. Modelling run times vary according to the size and complexity of the scenario that is being modelled. Results from the five test areas are summarized in Table 29 below.

Only one partner tested the effect of applying mitigation measures to model results and this showed the correct factor of reduction for the calculated surface water input loads for run-off and erosion. It also correctly showed no reduction of the input loads for drain flow.

	Scenario	Size	Scenario runs	Machine	Run time
Scania	Default, 1 crop	6,022 km^2, 81 polygons	340	High Spec	3.9 minutes
Scania	Detailed, 1 crop	6,022 km^2, 81 polygons	324	High Spec	1 hour
Lombardy Plain	Default, 2 crop(s)	13,500 km^2, 70 polygons	590	High Spec	11.7 minutes
Lombardy Plain	Detailed, 2 crop(s)	13,500 km^2, 242 polygons	2,410	High Spec	14.5 minutes
Denmark	Default, 1 crop	32,800 km^2 85 polygons	255	High Spec	(5 minutes)
Denmark	Detailed, 1 crop(s)	32,375 km^2 71 polygons	213	High Spec	(5 minutes)
England & Wales	Default 1 crop	176 km^2, 4 polygons	42	High Spec	20 seconds
England & Wales	Default 1 crop	176 km^2, 4 polygons	42	Moderate Spec	55 seconds
England & Wales	Default 1 crop	11,066 km^2, 72 polygons	304	High Spec	5.4 minutes
England & Wales	Default 1 crop	11,066 km^2, 72 polygons	304	Moderate Spec	10.2 minutes
England & Wales	Default 1 crop	82,518 km^2, 1,446 polygons	4,338	High Spec	2.74 hours
England & Wales	Default 1 crop	82,518 km^2, 1,446 polygons	4,338	Moderate Spec	4.53 hours
Slovenia	Default, 1 crop	20 273 km^2, 532 polygons	1,596	High Spec	76 sec

Table 29 -Modelling run times for different scenarios from the five test areas

2.3.5 The Communication and Reporting Module

All partners found the module easy to use and were able to visualize results both in map and table form for their scenarios, including the two detailed scenarios created with the user's own data. When using the module, loading of map legends is especially fast. However, the range of possible output results and formats can be confusing for inexperienced users and it is recommended that future development of the tool includes the addition of more comprehensive help routines to explain the data types, terms and percentages used in the legend(s).

2.4 Perspectives

The Beta testing phase carried out by the five partners was successful in identifying a range of bugs in the FOOT-NES Modules. This process is continuing and the latest version of the tool at the time of finishing the testing was 0.5.3417.38127. On May 19 2009 a new version of the FOOTPRINT tools (v. 0.6.1) became available. This replaces the former three installation files (.msi for FOOT-NES, FOOT-CRS and the Pesticide Scenario Manager) with a single installation file and makes the setting up of FOOT-NES considerably easier. However, the new version was not available in time for assessment during the beta-testing phase reported here. The latest version is v. 0.7.12, dated 19 January 2010.

Overall, the tool is quite complex. A basic knowledge of ArcGIS techniques is required and users need to take some time to familiarize themselves with the relationship between the various modules and the correct procedure to undertake a pesticide exposure assessment. They also need a very clear understanding of the different datasets that are required by the tool and the necessary format of folder and data file names. In particular, it is important to ensure that the paths (folder and file names) specified in the Data Management module are in a format compatible with ArcGIS, with no blank spaces in the names.

However, once this is completed and the modules are all operating, the tool appears to work well. The maximum run time for the most complex scenario used in the testing (4338 scenario runs for a crop covering 21% of all agricultural land in an area comprising over 70% of the agricultural land in England and Wales - 82,518 km^2) was 2.7 hours for a high specification machine and 4.5 hours for a moderate specification machine. Development work is continuing to improve these run times but it is still likely that running a pesticide application scenario for multiple crops and the whole of Europe will take one night to complete.

FOOT-NES is easiest to use with the ‘Default’ European-level data and scenarios that have been developed for it. To construct more detailed scenarios incorporating the user’s own local or regional data is more complicated and requires a good knowledge of GIS. It also requires use of the FOOTPRINT Soil Selector software or flow charts to correlate local soil types with the FOOTPRINT Soil Types. Although these tools include only basic terms, it is best if they are used by someone with background knowledge of soil science or users are helped by someone with such knowledge.

In summary, at this stage of development, the FOOT-NES tool is still at the beta testing stage, with additional testing necessary before it can be considered robust enough for public release. For the future, it is recommended that:

- A clear step-by-step User Manual is written to guide users through installation and operation of the tool.
- Further work is carried out to improve the ‘help’ routines associated with each module, especially explanation of the different types of results data that are selected in the Pesticide Scenario Manager and Modelling Module and presented in the Communication & Reporting Module.
- Internal error checking and associated warning messages are built into the tool to ensure that file and folder names have the correct format.
- A further schedule of systematic beta testing be developed to test the tool’s operation in different countries, crops and climates and to produce an estimate of the likely modelling running times for a range of specified scenarios, including some EU-wide runs.
- A full evaluation of the tool model predictions against monitoring data results is carried out for all five test areas once the FOOTPRINT modelling databases are complete.

CHAPTER 6 – CONCLUSIONS AND PERSPECTIVES

The FOOTPRINT project combined the expertise of 15 partners from 9 European countries for 3.5 years to develop methodologies and tools for pesticide risk assessment and management. Within the official project period from January 2006 to June 2009, the consortium produced a considerable amount of scientific output:

- The three FOOTPRINT tools operating at three different scales and addressing the needs of different environmental and agricultural user communities
- The FOOTPRINT agro-environmental scenarios
- The FOOTPRINT soil classification system (FOOTPRINT soil types, FOOTPRINT hydrologic groups, Flow Pathway Categories)
- Parameterisation methodologies for the pesticide fate models MACRO and PRZM
- The FOOTPRINT Pesticide Properties Database (PPDB)
- The FOOTPRINT SUGAR index
- 9 peer-reviewed papers (further papers are in preparation).

A start-up company FOOTWAYS was created by the FOOTPRINT coordinator and a leading scientist to ensure that the FOOTPRINT science and tools are supported in the long term. FOOTWAYS proposes to:

- provide long-term support and maintenance for the existing FOOTPRINT tools;
- offer training courses in the use of FOOT-FS, FOOT-CRS and FOOT-NES, to promote the widespread adoption of the FOOTPRINT tools;
- develop new, innovative tools which address inherent limitations of the FOOTPRINT tools identified during the project.

The three FOOTPRINT tools are expected to prove very valuable to support MS and EU policies related to the protection of water quality (Water Framework Directive and its daughter directives, drinking water legislations) or pesticide use (Directive on the Sustainable Use of Pesticides, new regulation on pesticide registration), which makes FOOTPRINT a key contributor towards a sustainable European agriculture. The three FOOTPRINT tools will be available publicly and free of charge on the FOOTPRINT website.

Although the FOOTPRINT project focused on pesticides, it is important to note that the FOOTPRINT work has potential applications for pollutants other than pesticides. For instance, the FOOTPRINT agro-environmental scenarios are model-independent and could be used to support risk assessments for nitrate, phosphorus, human and veterinary pharmaceuticals, or specific biocides.

Overall, many consider that FOOTPRINT has been a very successful project, and the former FOOTPRINT partners and FOOTWAYS will do their best to ensure the widespread and continuing use of the FOOTPRINT tools as well as other FOOTPRINT outputs.

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ANNEXES

FOOTPRINT scientific publications

The following scientific papers relate to work undertaken within FOOTPRINT. Electronic and paper reprints can be requested from www.eu-footprint.org

Jarvis N.J. (2007). A review of non-equilibrium water flow and solute transport in soil macropores: principles, controlling factors and consequences for water quality. *European Journal of Soil Science*, 58:523-546.

Abstract: This review discusses the causes and consequences of 'non-equilibrium' water flow and solute transport in large structural pores or macropores (root and earthworm channels, fissures and interaggregate voids). The experimental evidence suggests that pores larger than c. 0.3 mm in equivalent cylindrical diameter allow rapid non-equilibrium flow. Apart from their large size and continuity, this is also due to the presence of impermeable linings and coatings that restrict lateral mass exchange. Macropores also represent microsites in soil that are more biologically active, and often more chemically reactive than the bulk soil. However, sorption retardation during transport through such pores is weaker than in the bulk soil, due to their small surface areas and significant kinetic effects, especially in larger macropores. The potential for non-equilibrium water flow and solute transport at any site depends on the nature of the macropore network, which is determined by the factors of structure formation and degradation, including the abundance and activity of soil biota such as earthworms, soil properties (e.g. clay content), site factors (e.g. slope position, drying intensity, vegetation) and management (e.g. cropping, tillage, traffic). A conceptual model is proposed that summarizes these effects of site factors on the inherent potential for non-equilibrium water flow and solute transport in macropores. Initial and boundary conditions determine the extent to which this potential is realized. High rain intensities clearly increase the strength of non-equilibrium flow in macropores, but the effects of initial water content seem complex, due to the confounding effects of soil shrinkage and water repellency. The impacts of macropore flow on water quality are most significant for relatively immobile solutes that are foreign to the soil and whose effects on ecosystem and human health are pronounced even at small leached fractions (e.g. pesticides). The review concludes with a discussion of topics where process understanding is still lacking, and also suggests some potential applications of the considerable knowledge that has accumulated in recent decades.

Stenemo F. & Jarvis N.J. (2007). Accounting for uncertainty in pedotransfer functions in vulnerability assessments of pesticide leaching to groundwater. *Pest Management Science*, 63(9):867-875.

Abstract: A simulation tool for site-specific vulnerability assessments of pesticide leaching to groundwater was developed, based on the pesticide fate and transport model MACRO, parameterized using pedotransfer functions and reasonable worst-case parameter values. The effects of uncertainty in the pedotransfer functions on simulation results were examined for 48 combinations of soils, pesticides and application timings, by sampling pedotransfer function regression errors and propagating them through the simulation model in a Monte Carlo analysis. An uncertainty factor, fu, was derived, defined as the ratio between the concentration simulated with no errors, csim, and the 80th percentile concentration for the scenario. The pedotransfer function errors caused a large variation in simulation results, with fu ranging from 1.14 to 1440, with a median of 2.8. A non-linear relationship was found between fu and csim, which can be used to account for parameter uncertainty by correcting the simulated concentration, csim, to an estimated 80th percentile value. For fine-textured soils, the predictions were most sensitive to errors in the pedotransfer functions for two parameters regulating macropore flow (the saturated matrix hydraulic conductivity, Kb, and the effective diffusion pathlength, d) and two water retention function parameters (van Genuchten's N and a parameters). For coarse-textured soils, the model was also sensitive to errors in the exponent in the degradation water response function and the dispersivity, in addition to Kb, but showed little sensitivity to d. To reduce uncertainty in model predictions, improved pedotransfer functions for Kb, d,N and a would therefore be most useful.

Reichenberger S., Bach M., Skitschak A. & Frede H.-G. Mitigation strategies to reduce pesticide inputs into ground- and surface water and their effectiveness: a review. *The Science of the Total Environment*, 384:1-35.

Abstract: In this paper, the current knowledge on mitigation strategies to reduce pesticide inputs into surface water and groundwater, and their effectiveness when applied in practice is reviewed. Apart from their effectiveness in reducing pesticide inputs into groundand surface water, the mitigation measures identified in the literature are evaluated with respect to their practicability. Those measures considered both effective and feasible are recommended for implementing at the farm and catchment scale. Finally, recommendations for modelling are provided using the identified reduction efficiencies. Roughly 180 publications directly dealing with or being somehow related to mitigation of pesticide inputs into water bodies were examined. The effectiveness of grassed buffer strips located at the lower edges of fields has been demonstrated. However, this effectiveness is very variable, and the variability cannot be explained by strip width alone. Riparian buffer strips are most probably much less effective than edge-of-field buffer strips in reducing pesticide runoff and erosion inputs into surface

waters. Constructed wetlands are promising tools for mitigating pesticide inputs via runoff/erosion and drift into surface waters, but their effectiveness still has to be demonstrated for weakly and moderately sorbing compounds. Subsurface drains are an effective mitigation measure for pesticide runoff losses from slowly permeable soils with frequent waterlogging. For the pathways drainage and leaching, the only feasible mitigation measures are application rate reduction, product substitution and shift of the application date. There are many possible effective measures of spray drift reduction. While sufficient knowledge exists for suggesting default values for the efficiency of single drift mitigation measures, little information exists on the effect of the drift reduction efficiency of combinations of measures. More research on possible interactions between different drift mitigation measures and the resulting overall drift reduction efficiency is therefore indicated. Point-source inputs can be mitigated against by increasing awareness of the farmers with regard to pesticide handling and application, and encouraging them to implement loss-reducing measures of “best management practice”. In catchments dominated by diffuse inputs at least in some years, mitigation of point-source inputs alone may not be sufficient to reduce pesticide loads/concentrations in water bodies to an acceptable level.

Blenkinsop S., Fowler H.J., Dubus I.G., Nolan B.T. & Hollis J.M. (2008). Developing climatic scenarios for pesticide fate modelling in Europe. *Environmental Pollution*, 154:219-231.

Abstract: A climatic classification for Europe suitable for pesticide fate modelling was constructed using a 3-stage process involving the identification of key climatic variables, the extraction of the dominant modes of spatial variability in those variables and the use of k-means clustering to identify regions with similar climates. The procedure identified 16 coherent zones that reflect the variability of climate across Europe whilst maintaining a manageable number of zones for subsequent modelling studies. An analysis of basic climatic parameters for each zone demonstrates the success of the scheme in identifying distinct climatic regions. Objective criteria were used to identify one representative 26-year daily meteorological series from a European dataset for each zone. The representativeness of each series was then verified against the zonal classi- fications. These new FOOTPRINT climate zones provide a state-of-the-art objective classification of European climate complete with representative daily data that are suitable for use in pesticide fate modelling.

Barriuso E., Benoit P. & Dubus I.G. (2008). The formation of pesticide bound residues in soil: magnitude, controlling factors and reversibility. *Environmental Science & Technology*, in press.

Abstract: The analysis of the coherent data on non-extractable (bound) residues (NER) from the literature and EU pesticide registration dossiers allows the identification of general trends, in spite of the large variability and heterogeneity of data. About 50% of the pesticides reviewed exhibit a low proportion of NER (less than 30% of the initial amount) while only 12% of pesticides have a proportion of NER exceeding 70%. The lowest proportion of NER was found for dinitroanilines (< 20%) and the largest value was obtained for carbamates, and in particular dithiocarbamates. The presence of chemical reactive groups, such as aniline or phenol, tends to yield a larger proportion of NER. NER originating from N-heteroatomic ring were found to be lower than from phenyl-ring structures. Among the environmental factors affecting the formation of NER, microbial activity has a direct and significant effect. Concerning the NER uptake or their bioavailability, consistent data suggest that only a small percentage of the total amounts of NER can be released. The analysis of NER formation kinetics showed that incubation experiments are often stopped too early to allow a correct evaluation of the NER maturation phase. There is therefore a need for longer term experiments to evaluate the tail of the NER formation kinetics. Still, the heterogeneity of the NER data between pesticides and for specific pesticides calls for great care in the interpretation of the data and their generalisation.

Nolan B.T., Dubus I.G., Surdyk N., Fowler H.J., Burton A., Hollis J.M., Reichenberger S. & Jarvis N.J. (2008). Identification of key climatic factors regulating the transport of pesticides in leaching and to tile drains. *Pest Management Science*, in press.

Abstract: We identified key climatic factors influencing the fate of pesticides in the environment as part of an ongoing risk assessment for the European Union. Climatic zonations for fate modelling were previously based on average annual temperature and rainfall. Other climate characteristics, such as the timing of rainfall in relation to pesticide application, may be more critical. We simulated the fate of three pesticides, nine contrasting soil types, two application periods, five application dates, and six climatic data series using the pesticide leaching model MACRO. The climatic data were then characterized in detail with regard to rainfall and temperature patterns before and after pesticide application. Predicted cumulative pesticide loads were analyzed and related to climatic variables using statistical methods. Soil type was a dominant factor controlling pesticide loss in both leaching and drainage scenarios. Clay soils were consistently associated with upper-quartile pesticide losses (>0.046 mg/m2 for leaching and 0.042 mg/m2 for drainage). Winter rainfall influenced losses of less mobile and more persistent compounds, while short-term rainfall and temperature controlled the more mobile pesticides. Climate interacted strongly with soil type under both leaching and drainage scenarios. The influence of short-term climatic variables

and the timing of extreme events in relation to pesticide application were greater for drainage scenarios than for leaching, which is consistent with the rapid transport of pesticide via macropores in fine-textured soils. Climatic factors identified here are being used to refine climatic zonations representing the European Union.

Centofanti T., Hollis J.M., Blenkinsop S., Fowler H.J., Truckell I., Dubus I.G. & Reichenberger S. (2008). Development of agro-environmental scenarios to support pestcide risk assessment in Europe.*The Science of the Total Environment*, 407:574-588.

<u>Abstract:</u> This paper describes work carried out within the EU-funded FOOTPRINT project to characterize the diversity of European agricultural and environmental conditions with respect to parameters which most influence the environmental fate of pesticides. Pan-European datasets for soils, climate, land cover and cropping were intersected, using GIS, to identify the full range of unique combinations of climate, soil and crop types which characterize European agriculture. The resulting FOOTPRINT European agro-environmental dataset constitutes a large number of polygons (approximately 1,700,000) with attribute data files for i) area fractions of annual crops related to each arable-type polygon (as an indicator of its probability of occurrence); and, ii) area fractions of each soil type in each polygon (as an indicator of its probability of occurrence). A total of 25,044 unique combinations of climate zones, agricultural land cover classes, administrative units and soil map units were identified. The same soil/crop combinations occur in many polygons which have the same climate while the fractions of the soils and arable crops are different. The number of unique combinations of climate, soil and agricultural land cover class is therefore only 7961. 26-year daily meteorological data, soil profile characteristics and crop management features were associated with each unique combination. The agro-environmental scenarios developed can be used to underpin the parameterization of environmental fate models for pesticides and should also have relevance for other agricultural pollutants. The implications for the improvement and further development of risk assessment procedures for pesticides are discussed.

Jarvis N.J., Moyes J., Hollis J.M., Reichenberger S., Lindahl A. & Dubus I.G. (2009). A conceptual model of soil susceptibility to macropore flow. *Vadose Zone Journal*, in press.

<u>Abstract:</u> The extent to which a fast, non-equilibrium and highly transient pore-scale process such as macropore flow can be predicted is very often debated, although little research has been conducted to investigate this issue. The validity of approaches to ‘upscaling’ transport predictions from pore through Darcy to landscape scales critically depends on the answer to this question. In this paper we develop and describe a simple conceptual model of soil susceptibility to macropore flow, based on a synthesis of existing experimental information. The conceptual model takes the form of a decision tree, which classifies soil horizons into one of four susceptibility classes on the basis of easily available site and soil factors. The model was tested against an independent database of tracer breakthrough experiments on

undisturbed soil columns collated from the literature (n=52), using the pore volumes drained at peak solute concentration tp as a measure of the strength of macropore flow. Analysis of variance for tp as a function of susceptibility class showed that the overall model was significant. A significant proportion of the residual variation in tp could be attributed to variation in clay content within one of the susceptibility classes. Some important sources of experimental error were also identified which may account for much of the remaining unexplained variation. It is concluded that macropore flow is predictable to a sufficient degree from easily available soil properties and site factors. The simple classification tree developed in this paper could be used to support hydro-pedological approaches to quantifying the spatial distribution of contaminant leaching at the landscape scale, by providing the basis for class pedotransfer functions to estimate model parameters related to macropore flow. Such an approach has been implemented in the European project FOOTPRINT.

Lindahl A.I., Dubus I.G. & Jarvis N.J. (2009). Site classification to predict the abundance of the deep-burrowing earthworm Lumbricus terrestris L. Vadose Zone Journal, in press.

Abstract: Channels made by deep-burrowing ('anecic') earthworms are known to strongly affect soil water flow and increase the leaching risk of agricultural pollutants. A classification tree that predicts the abundance of the anecic earthworm Lumbricus terrestris L. from readily available survey information (land use, management practices and soil texture) was derived from literature data (n = 86). The most important factors favouring Lumbricus terrestris L. were perennial land use, no-till arable cropping, organic additions (i.e. manure) and medium-textured soil. The classification scheme correctly predicted earthworm abundance for 71% of the studies in the database. Among other potential applications, the classification tree could be used to identify areas at risk from groundwater pollution in agricultural landscapes and to support catchment and regional-scale models of contaminant leaching in the vadose zone.