Wettelijke Onderzoekstaken Natuur & Milieu

SWASH Manual 5.3

User's Guide version 5

| WOt-technical report 36

F. van den Berg, W.H.J. Beltman, P.I. Adriaanse, A. de Jong & J.A. te Roller

WAGENINGEN UR
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Abstract
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SWASH (Surface WAter Scenarios Help) assists the user in calculating pesticide exposure concentrations using the EU FOCUS Surface Water Scenarios. Calculating exposure concentration is part of the obligatory evaluation procedure to place an active substance in a registry according to the new EU Regulation 1107/2009. SWASH encompasses: (i) FOCUS Drift Calculator, calculating pesticide entries through spray drift deposition, (ii) PRZM-3, calculating pesticide entries through run-off, (iii) MACRO, calculating pesticide entries through drainage and (iv) TOXSWA, calculating the behaviour of pesticides in small surface waters. It is linked to SPIN, a pesticide properties tool, and prepares input for the PRZM, MACRO and TOXSWA models. Via the SWASH shell the user can enter the shells of the other models to perform the PRZM or MACRO model runs needed to assess the fate of the substance in the FOCUS surface water systems using TOXSWA.

Key words: ditch, drainage, drift, exposure assessment, pesticide, pond, run-off, scenario, stream, surface water, FOCUS, MACRO, PRZM, SPIN, TOXSWA

Referaat
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SWASH (Surface WAter Scenarios Help) ondersteunt de gebruiker om blootstellingsconcentraties van gewasbeschermingsmiddelen in de EU FOCUS oppervlaktewaterscenario's te berekenen. De berekening is onderdeel van de verplichte evaluatieprocedure om een actieve stof te plaatsen in een register volgens EU Richtlijn 1107/2009. SWASH omvat vijf verschillende instrumenten en modellen: (i) FOCUS Drift Calculator berekent de belasting van gewasbeschermingsmiddelen door driftdepositie, (ii) PRZM-3 berekent de belasting van gewasbeschermingsmiddelen door afspoeling, (iii) MACRO berekent de belasting van gewasbeschermingsmiddelen als gevolg van uitspoeling, (iv) TOXSWA berekent het gedrag van gewasbeschermingsmiddelen in kleine watersystemen, en (v) SPIN is een centrale database voor opslag en aanpassen van eigenschappen van gewasbeschermings-middelen. SWASH zet de invoergegevens klaar voor de modellen PRZM, MACRO en TOXSWA. Via de SWASH-schil kan de gebruiker de schillen van PRZM en MACRO binnengaan om de berekeningen uit te voeren die nodig zijn om het gedrag van de stof in de FOCUS oppervlaktewatersystemen te simuleren met TOXSWA.

Trefwoorden: beek, blootstellingsbeoordeling, drainage, drift, gewasbeschermingsmiddel, oppervlaktewater poel, run-off, scenario, sloot, FOCUS, MACRO, PRZM, SPIN, TOXSWA

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Preface

End of 1997 the FOCUS Surface Water Scenarios Working Group started its activities. The Group developed a tiered approach to estimate pesticide exposure concentrations in surface water, which was submitted to the Working Group on Pesticide Legislation of the European Union. Since 2003, the calculated concentrations using the FOCUS Surface Water Scenarios have become part of the EU review process for plant protection products according to EU Directive 1107/2009. In the proposed Step 3 calculations a tool for drift assessment and three models are combined to calculate exposure concentrations in the various types of surface water bodies. To promote an easy and consistent way of calculation, an overall user-friendly software shell was developed to guide the user through the needed calculations and to maintain a central pesticide database.

Alterra took the initiative to realise the user-friendly shell SWASH, acronym for Surface WAter Scenarios Help, and was developed by Erik van den Berg and Paulien Adriaanse from the Environmental Risk Assessment team of Alterra Wageningen UR, in co-operation with Johnny te Roller and Daniel van Kraalingen from the Earth Informatics team of Alterra Wageningen UR (1999 - 2003). Nick Jarvis (Swedish University of Agricultural Science, Sweden) for MACRO, Mark Russell (Dupont Crop Protection, USA) and Mark Cheplick (Waterborne Environmental, USA) for PRZM collaborated closely with them to realise the communication between the models and the SWASH database. Denis Yon (Dow Agrosciences, UK) and Mark Russell developed together the FOCUS drift calculator (FOCUS, 2001) and this instrument has also been included in SWASH.

The first version of SWASH, FOCUS_SWASH_1.1, was financed for 25% by the ECPA (European Crop Protection Agency), 25% by the Dutch Ministry for Agriculture, Fisheries and Nature Management and 50% by DG SanCO from the EU. All other work has been financed by the Dutch Ministry of Economic affairs (up to 2010 by the Dutch Ministry of Agriculture, Nature and Food Quality).

Since the first release in 2001, four updates of SWASH have been made, i.e. FOCUS_SWASH 2.1 (2008), FOCUS_SWASH 3.1 (2009), FOCUS_SWASH 4.2 (not released) and recently FOCUS_SWASH 5.3 (2015).

The current document is the user's manual of the latest version of SWASH: FOCUS_SWASH_5.3. This document is an updated version of the SWASH 4.2 manual (Fait *et al.*, 2013). The current document considers the changes made in the new version of SWASH to support the metabolite option in the new FOCUSTOXSWA 4.4.3 version.

The SWASH developers hope that the SWASH users will profit from their efforts and that the users will be able to calculate in a straightforward and reproducible way the pesticide exposure concentrations in all Step 3 scenarios.

Additionally, a more technical document has been written (Te Roller *et al*., 2015), explaining the technical design of the SWASH database, the SWASH user interface and the communication and installation procedures.

Contents

Summary

A tiered approach has been developed to assess pesticide exposure of aquatic organisms in the EU FOCUS scenarios for surface waters. In Step 3 of the tiered approach, a drift assessment tool, two models to calculate pesticide input into the surface water and a model to assess the fate in surface water have to be run in sequence. The drift assessment tool and the pesticide fate models have been developed separately targeting a specific aspect relevant to the assessment.

These are:
- Drift Calculator, calculating pesticide deposition onto surface water due to spray drift;
- FOCUS_PRZM_SW_4.3.1, calculating pesticide entry into surface water through run-off;
- FOCUS_MACRO_5.5.4, calculating pesticide entry into surface water through drainage;
- FOCUS_TOXSWA_4.4.3, calculating the fate of pesticides and their metabolites in surface waters.

To facilitate the calculation of exposure concentrations at the Step 3 level a software tool has been developed: SWASH, acronym for Surface WAter Scenarios Help. It is an overall user-friendly shell, encompassing the tool to assess deposition due to spray drift and the three models involved in Step 3 calculations.

The main functionalities of SWASH are:
- Provision of an overview of all Step 3 FOCUS runs required for use of a specific pesticide on a specific crop as specified by the user;
- Calculation of spray drift deposition onto various receiving water bodies with the FOCUS Drift Calculator; and
- Preparation of all input needed for the MACRO, PRZM and TOXSWA models.

In addition, SWASH provides information on the FOCUS Surface Water Scenarios.

Finally, SWASH provides a directory structure for the various models and their input and output to enable a smooth and correct communication between the Drift Calculator, MACRO and TOXSWA and between the Drift Calculator, PRZM and TOXSWA.

After creating a project with FOCUS runs in SWASH, the user has to perform simulations with the individual models: PRZM, MACRO and TOXSWA. SWASH does not execute model runs, but provides guidance, helps the user to determine which runs need to be performed for pesticide applications to various crops, and defines projects and runs for MACRO, PRZM and TOXSWA that can be selected for execution after starting the corresponding shells.

Since SWASH version 4.2, the substance properties module is removed. SWASH is now directly linked to SPIN (Substance Plug In). SPIN is a new software tool, consisting of a shell for entry of substance properties and a separate database for storage of the substance data.

Samenvatting

Een getrapte benadering is ontwikkeld om de blootstelling van aquatische organismen aan gewasbeschermingsmiddelen in de EU FOCUS-oppervlaktewaterscenario's te kunnen vaststellen. In Stap 3 van deze getrapte benadering dienen een instrument om drift vast te stellen, twee modellen om de belasting van het oppervlaktewater te berekenen en een model om het gedrag van het gewasbeschermingsmiddel daarvoor in de juiste volgorde te berekenen en aansluitend op elkaar te laten draaien. Het instrument om drift te bepalen en de modellen voor het gedrag van gewasbeschermingsmiddelen zijn apart ontwikkeld met voor elk als doel een specifiek onderdeel van de beoordeling. Dat waren:

- Drift Calculator, om de depositie op het oppervlaktewater als gevolg van drift te berekenen;
- FOCUS_PRZM_SW_4.3.1, om de belasting van het oppervlaktewater via run-off te berekenen;
- FOCUS_MACRO_5.5.4, om de belasting van het oppervlaktewater via drains te berekenen;
- FOCUS_TOXSWA_4.4.3, om het gedrag van de actieve stoffen en hun metabolieten in oppervlaktewater te berekenen.

Om de berekening van de blootstellingsconcentratie voor Stap 3 te vergemakkelijken, is een instrument ontwikkeld: SWASH, acronym voor Surface WAter Scenarios Help. Het is een overkoepelende gebruikersvriendelijke schil, die zowel het instrument voor de bepaling van de depositie als gevolg van spuitdrift als de modellen omvat die gebruikt worden om Stap 3 te berekenen. De belangrijkste functionaliteiten van SWASH zijn:

- Het bieden van een overzicht van alle Stap 3 FOCUS-runs voor het gebruik van een specifiek gewasbeschermingsmiddel op een specifiek gewas zoals de gebruiker dat heeft gedefinieerd;
- Berekening van de depositie op de verschillende ontvangende oppervlaktewatersystemen als gevolg van spuitdrift met de FOCUS Drift Calculator;
- Aanmaken van alle invoer nodig voor de MACRO, PRZM en TOXSWA.

Bovendien geeft SWASH ook nog informatie over de FOCUS Oppervlaktewater Scenario's.

Tot slot biedt SWASH een bestandsstructuur voor de verschillende modellen en hun invoer en uitvoer om daarmee een soepele en correcte communicatie mogelijk te maken tussen de Drift Calculator, MACRO en TOXSWA en tussen de Drift Calculator, PRZM en TOXSWA.

Na het maken van een project met FOCUS-runs in SWASH, dient de gebruiker simulaties uit te voeren met de individuele modellen: PRZM, MACRO and TOXSWA. SWASH voert geen modelruns uit, maar biedt richtlijnen en helpt de gebruiker om te bepalen welke runs uitgevoerd moeten worden voor toepassingen van gewasbeschermingsmiddelen in de verschillende gewassen en definieert projecten en runs voor MACRO, PRZM en TOXSWA die voor uitvoering geselecteerd kunnen worden na het starten van de corresponderende schil.

Sinds SWASH versie 4.2 is de module met de stofgegevens geen onderdeel meer van SWASH. SWASH is nu direct gekoppeld aan SPIN (Substance Plug In). SPIN is een nieuw instrument, dat bestaat uit een schil voor het invoeren van stofgegevens en een aparte database waarin de stofgegevens worden opgeslagen.

1 Introduction

Spray drift, drainage and run-off are three major routes of pesticide entry into surface waters. Using spray-drift deposition tables and the MACRO, PRZM and TOXSWA models the exposure concentrations in surface waters can be assessed. Exposure scenarios have been developed as part of the EU evaluation process under 1107/2009 (FOCUS, 2001). To carry out these exposure assessments scenarios for surface waters, a drift assessment tool and two pesticide fate models have to be run in the correct sequence (Figure 1.1). The drift assessment tool and the pesticide fate models have been developed separately targeting a specific aspect relevant to the assessment. These are:

- Drift Calculator, calculating pesticide deposition due to spray drift;
- FOCUS_PRZM_SW_4.3.1, calculating pesticide entry into surface water through run-off;
- FOCUS_MACRO_5.5.4, calculating pesticide entry into surface water through drainage;
- FOCUS_TOXSWA_4.4.3, calculating the fate of pesticides and their metabolites in surface waters.

In the FOCUS Surface Water Scenarios it has been assumed that pesticides enter surface water via two entry pathways only: deposition due to spray drift, plus either drainage or run-off. In total ten FOCUS scenarios have been defined: six drainage scenarios and four run-off scenarios.

The MACRO model (Jarvis, 1994; Jarvis & Larsson, 1998) describes the behaviour of pesticides in soils with and without macro-pores, considering transport by convection and diffusion through the liquid phase, sorption and transformation. FOCUS_MACRO version 5.5.3 was released in 2012. This version included the MACRO model version 5.2 with improved numerical routines for water flow and solute transport, and a replacement of the Brooks-Corey equation by the Van Genuchten equation. In 2015 a new version was released, version 5.5.4, in which the exponent for the effect of water content on transformation is adapted. MACRO is able to simulate the behaviour of one metabolite in soil after the simulation run for the parent compound has been completed.

The PRZM model (Carsel *et al*., 1998) is a one-dimensional model that simulates chemical movement in unsaturated soil systems within and immediately below the root zone. It calculates run-off and soil erosion into surface water for the FOCUS scenarios. The calculation is based upon the USDA Soil Conservation Service curve number methodology and several variations of the Universal Soil Loss Equation. In 2012 PRZM version 3.1.1. was released In this version amendments were made (e.g. technical improvements in PRZM run-off representation). In 2015 a new version was released, version 4.3.1, in which some pesticide input ranges were adapted. PRZM can describe three transformation schemes and up to two metabolites: 1) a parent with one metabolite, 2) a parent with two sequential metabolites and 3) a parent with two metabolites.

The TOXSWA model describes the behaviour of pesticides in small water bodies (Adriaanse, 1997). Processes considered are sorption, transport, volatilisation and transformation. FOCUS_TOXSWA 1.1.1 (FOCUS, 2001, Chapter 4 and Appendix L) handles transient hydrology and pesticide fluxes resulting from surface run-off, drainage and pesticide input from the upstream catchment basin. In this way FOCUS_TOXSWA_1.1.1 is able to simulate the flow dynamics in the edge-of-field water body in a realistic way. In 2005, FOCUS_TOXSWA_2.2.1 has been released (Beltman *et al.*, 2006). This version contains a Help utility and all reported bugs for FOCUS_TOXSWA_1.1.1 and later have been repaired. In 2009 a Windows Vista compatible version of FOCUS_TOXSWA was released: FOCUS_TOXSWA version 3.3.1. In 2015 FOCUS_TOXSWA 4.4.3 was released, enabling the simulation of metabolites formed in water and formed in sediment (Beltman *et al.*, 2014).

To assist the users of the FOCUS Surface Water Scenarios at the Step 3 level the software package FOCUS_SWASH has been developed. SWASH, the acronym for Surface WAter Scenarios Help, is an overall user-friendly shell, managing the communication and data transfer between three models involved in Step 3 calculations, using also the SPIN substances tool (Figure 1.1). The aims for the development of SWASH were to maintain a central pesticide properties database (now implemented in

SPIN), to provide an overview of all Step 3 FOCUS runs required for use of a specific pesticide on a specific crop as specified by the user, to calculate the spray drift deposition onto various receiving water bodies and to prepare all input needed for the MACRO, PRZM and TOXSWA models. The new version of FOCUS_SWASH is compatible with the new FOCUS_TOXSWA version, i.e. v4.4.3, which includes an option to consider metabolites formed in water and in sediment.

In Chapter 2 guidance is given on the use of SWASH. In Chapter 3 information is given on the installation of the software package and getting started to use SWASH.

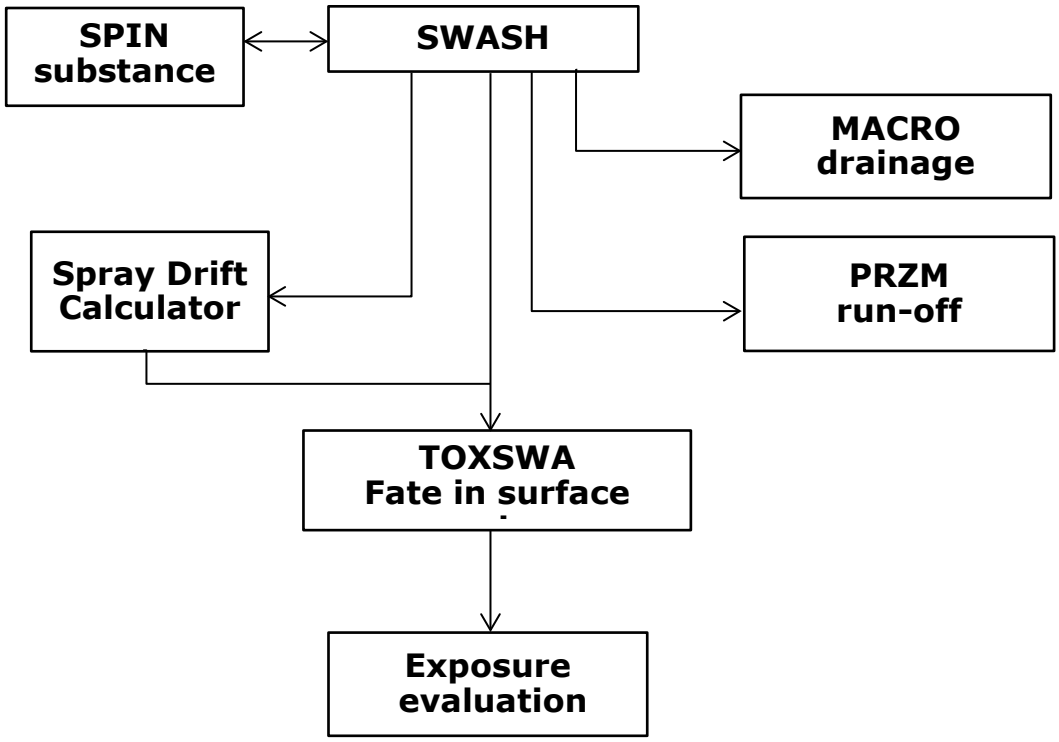

Figure 1.1. Sequence of tools and models used to calculate pesticide exposure in the proposed Step 3 EU FOCUS Surface Water Scenarios.

The improvements made in FOCUS_SWASH 5.3 are:

1. The Microsoft Access database (part of versions 1.1, 2.1 and 3.1) has been replaced by a Firebird database, in the past several problems occurred related to Microsoft Office versions. With the new database these kinds of problems are not expected to occur anymore.
2. A separate tool for pesticide properties, SPIN (Substance Properties plug IN), consisting of a shell and a database, is coupled to SWASH.
3. The handling of soil, water and sediment metabolites is facilitated. The new version of FOCUS_TOXSWA can handle metabolite formation in water and sediment. Therefore the handling of metabolites in SWASH is enabled.
4. The automatic calculation of correction factors for primary water metabolites formed in the upstream catchment of streams (Adriaanse *et al*., 2014).

2 User's guide for the SWASH User interface

Handling of the FOCUS Surface Water Scenarios is complex. Three different models, i.e. MACRO, PRZM and TOXSWA, and the Drift Calculator need to be used to assess the exposure concentrations of pesticides in surface waters that result from a pesticide loading via drift, drainage and run-off. The SWASH software package has been developed be able to execute FOCUS runs in an easy and user-friendly manner. In this chapter, an explanation is given on the functionalities of SWASH and guidance is given on the use of SWASH in evaluating the fate of a substance in surface waters using the FOCUS scenarios. First, the user is introduced to the tasks SWASH can perform. The possibilities to create projects and runs are explained and the basic use of the substance tool SPIN is shown using figures with presentations of the forms the user will see on the screen when working with SWASH. In the second part of this chapter an overview of the information in SWASH about the FOCUS Surface Water Scenarios is given.

2.1 The Main Screen - Actions

2.1.1 General

The main screen consists of two parts, namely 'Actions' and 'Information'. In the 'Actions' part the user undertakes activities with concrete results, i.e. the SWASH database is updated or projects and runs are created. The first part - 'Actions' - is displayed after clicking on the 'Actions' tab as shown in Figure 2.1.

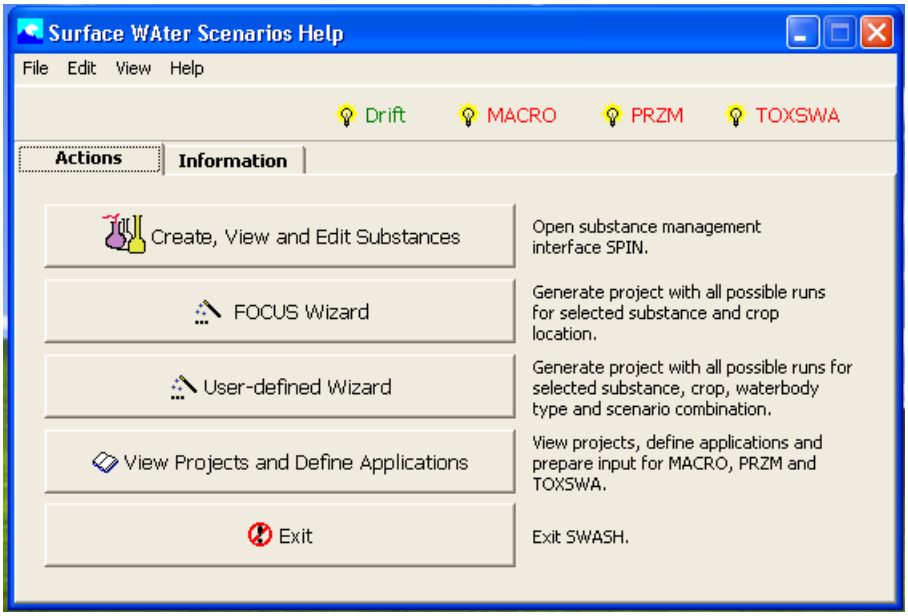

Figure 2.1. The main screen of the SWASH interface with the 'Actions' tab displayed.

The 'Actions' page contains five buttons and the function of the buttons will be briefly described here, but in more detail in the corresponding section of this chapter.

The button 'Create, View and Edit Substances' gives access to the SPIN database, where the user can enter new substances or modify the properties of substances already present in the database (see Annex 1). Four example substances, using the default properties, defined by the FOCUS Surface Water Group, are available in the database upon installation. The properties of these substances are fixed and cannot be modified.

The button 'FOCUS wizard' gives the user the possibility to easily create and execute FOCUS runs for a specific substance – crop combination. An overview as well as a report will be created for all those runs. The runs are organised in projects; for each substance – crop combination a separate project will be created. This wizard provides the user with all standard Step 3 runs for a specific substance-crop combination.

The button 'User-defined wizard' gives the user more freedom in selecting scenarios and crops for which runs have to be created. Using this wizard all possible FOCUS runs for a selected substance, one run for each scenario – crop – water body type combination can be created and put into a single project.

The button 'View Projects and Define Applications' presents the overview of the runs in all projects and allows the user to define or modify the application pattern for each run. For the runs in each project, the user can decide if project output has to be created. The project output consists of the creation of input for MACRO, PRZM, and TOXSWA for those runs selected by the user. The user can also print a text report on the specifications of the runs in a project (See Section 2.1.5).

Using the 'Exit' button, the user can end a SWASH session.

The buttons on the upper right corner of the screen, i.e. 'Drift', 'MACRO', 'PRZM' and 'TOXSWA' give the user a direct link to the Drift calculator and to the shells of the three FOCUS surface water models.

In the Information part of the main screen of SWASH the user is only informed about certain aspects of Step 3 exposure assessments, but no changes are made in the database, or input prepared for the other models. The Information part will be described in more detail in Section 2.2.

2.1.2 Substances, connection to SPIN

SWASH is linked to SPIN, a database that maintains all the substances and their properties., The main window of SPIN is shown in Figure 2.2. A detailed description of SPIN is given in the SPIN user manual (Van Kraalingen *et al.,* 2013).

Four example substances, defined by the FOCUS Surface Water Working Group, are available in the SPIN database upon installation (EXSW6, EXSW6m, EXSWA, EXSWH). EX stands for example, SW for surface water). These compounds correspond to the FOCUS surface water example compounds, e.g. EXSW6 corresponds to 6_sw). The properties of these substances are fixed and cannot be modified. The parameterization of the example substances was kept as suggested by the FOCUS Surface Water Working Group (FOCUS, 2001).

New values were adopted by EFSA for the Arrhenius activation energy (used in TOXSWA), the Q10 factor (used in PRZM), and the alpha factor (used in MACRO). Therefore, the example substance EXSW0 has been added to SPIN and parameterized according to new default values (EFSA, 2007).

The user can enter new substances or modify the properties of a substance already present in SPIN. Substances entered in SPIN are automatically transferred to the database of MACRO and to the substance file of PRZM after SPIN is closed. TOXSWA accesses the SPIN database directly.

To create a new substance for FOCUS surface waters calculations, it is advised to copy one of the example substances EXSW0 and change the values of the properties into the values of the new substance. By using the example substance EXSW0 all the EFSA default values will be set properly.

All the parameters required for running the FOCUS surface water models have to be entered, otherwise the substance (either a parent or a metabolite) will appear in SWASH as 'incomplete' and it is not be possible to run a project containing a substance for which not all necessary data have been specified.

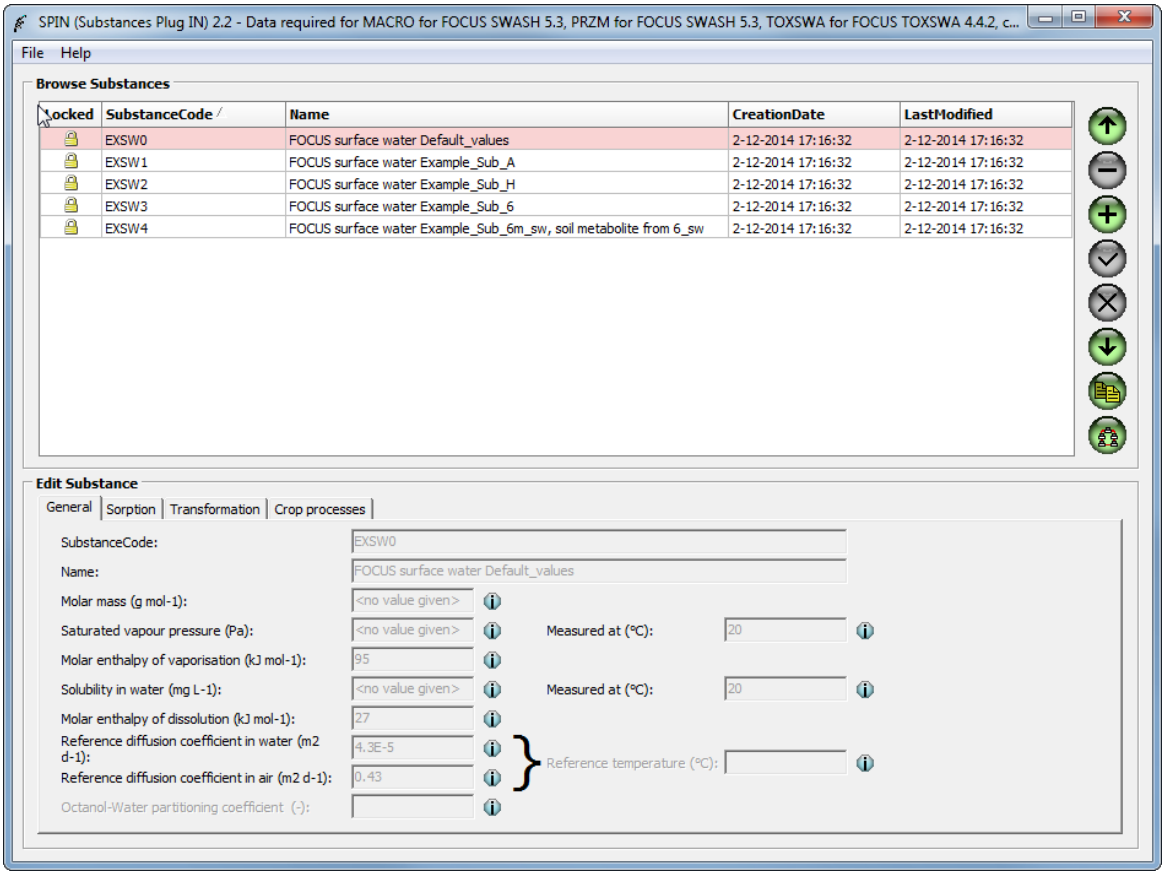

Figure 2.2. SPIN main window.

The user has to be aware that SWASH does not give any warnings in case a substance parameter is modified. This is important when changing a parameter of a substance that has already been run with the models. However, the values used in the TOXSWA run are listed in the summary file of TOXSWA.

The handling of metabolite substances is described in Section 2.1.6.

2.1.3 The FOCUS wizard

The FOCUS wizard is a tool to assist the user to generate all the runs needed for a specific substance – crop combination and to create a report with an overview of these runs. The wizard will select all drainage and run-off scenarios for which the crop is relevant. After clicking on the button 'FOCUS wizard' on the main window, the form shown in Figure 2.3 is shown. The user has to fill this form with the following information:

- The name of the project.
- The description of the project.
- The project path; this directory is created to contain all input and output files related to this project; it is recommended to keep such directories for future reference.
- The substance to be assessed; the substance can be selected from the list of substances present in SPIN. The list is shown by clicking on the button with the arrow on the right-hand side of the 'Substance' field. Here it is possible to check whether a substance is complete, incomplete or ambiguous. FOCUS runs can only be performed for substances which are complete and unambiguous (see Section 2.1.6).
- The crop for which the substance will be used; the crop can be selected from the list of crops present in the database. The list is shown by clicking on the button with the arrow on the right-hand side of the 'Crop' field.

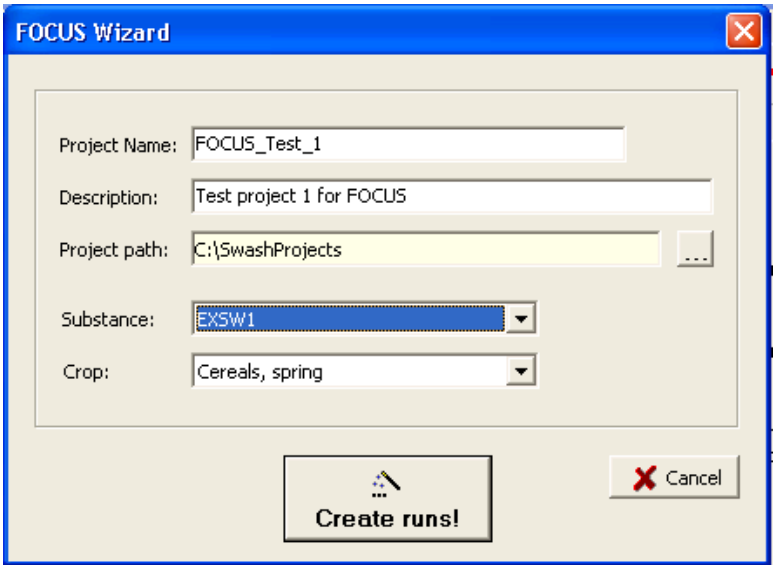

Figure 2.3. The FOCUS wizard.

After the form has been completed, the user clicks on the 'Create runs' button and all valid FOCUS runs for the selected crop are generated and put into a single project with the name specified in the field 'Project Name'. When the wizard is ready, in a separate window the user gets information on how many runs have been created. After clicking on 'OK' the main window of SWASH is shown again. It should be noted that the directory specified in the field 'Project path' is empty after completing the procedure of the FOCUS wizard. Subdirectories and files will only be created after exporting data to PRZM, MACRO and TOXSWA (See Section 2.1.5).

The user can get an overview of the runs created by clicking on the button 'View projects and define applications' (Figure 2.1). An example of the 'Overview of composed projects' window of SWASH is shown in Figure 2.4. In the upper part of the window all the projects created in SWASH are listed. In the lower part of the window the runs created for the selected project are listed. After clicking on the 'View and Edit applications button, the window shown in Figure 2.5 appears on the screen.

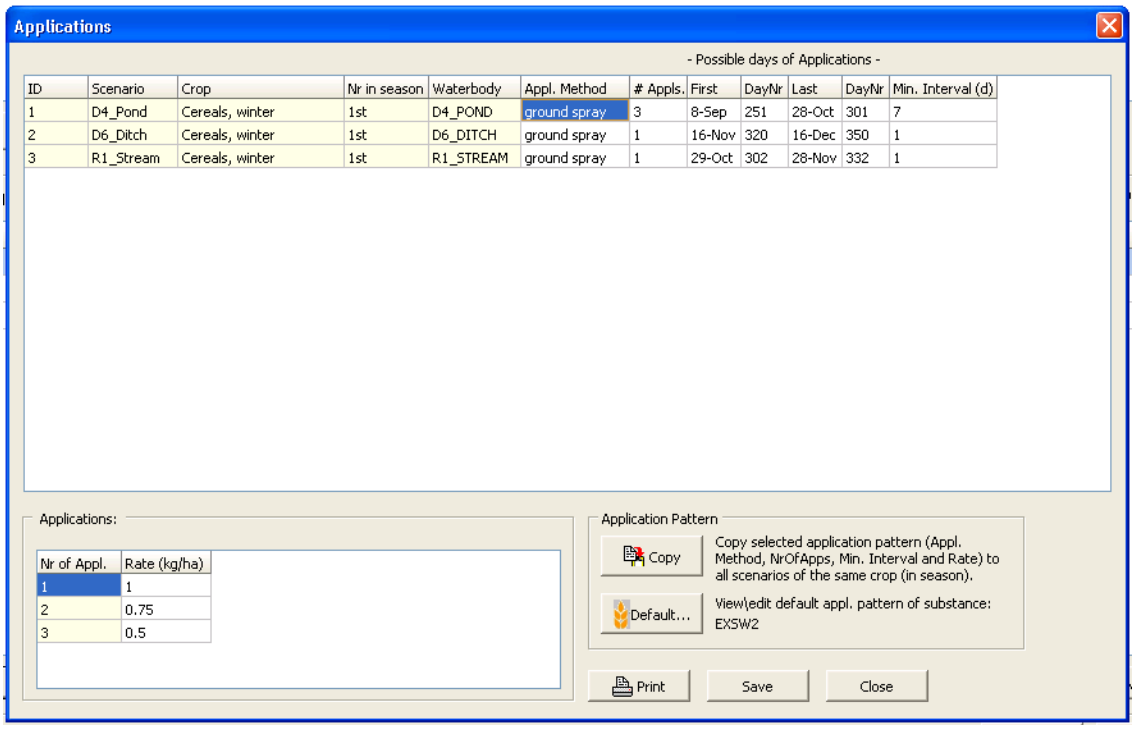

Figure 2.4. Overview of the projects and the runs in the selected project.

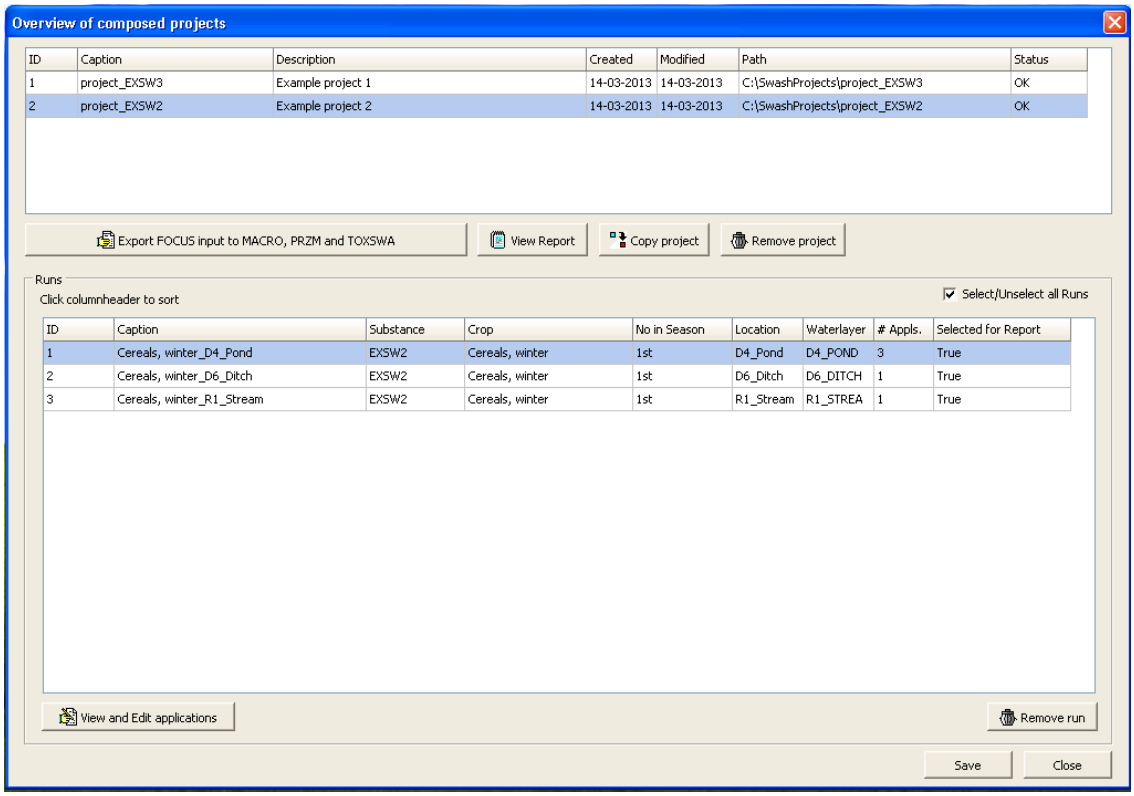

Figure 2.5. Detailed description of the runs in a project.

The forms shown in Figure 2.4 and Figure 2.5 are explained in detail in Section 2.1.5.

It should be noted that the user has to check the application input data. The user cannot specify the day of application himself, but only the boundary conditions, such as the first possible day of application and the last possible day of application. The exact date of the application is calculated by the tool called 'PAT'- Pesticide Application Timer. This tool is part of the software package of MACRO and PRZM, and the determination of the day of application is done using a standard procedure (FOCUS, 2001). The date of application is also needed in TOXSWA to specify the loading of pesticide by drift. For FOCUS drainage scenarios, the date of application is read by TOXSWA from the MACRO output for TOXSWA (header of .m2t file) and for FOCUS run-off scenarios the date is read from the PRZM output for TOXSWA (header in .p2t file).

Changed in FOCUS_SWASH 4.2 compared to former versions is that the run ID attributed to a run is only a number now, whilst before the run ID included some characters indicating what type of waterbody (pond, ditch or stream) and what type of substance (parent or metabolite) was simulated. Now the ID number can differ from the number indicated in the name of the m2t file (MACRO) or the p2t file (PRZM). For Step 3 runs in the TOXSWA input file (txw file) or summary output file can be found which m2t or p2t file has been used in the TOXSWA simulation.

2.1.4 The User-Defined wizard

After clicking on the button 'User-defined Wizard' on the main window, the first form of the Wizard is displayed on the screen. On this form, shown in Figure 2.6, the user has to select the substance for which he/she wants to do FOCUS runs. The user can select a substance from the list of substances present in the database by clicking on the arrow on the right-hand side of the 'Substance' field. The substances available in the database are shown. If a substance is ' incomplete' or 'ambiguous' for use in FOCUS scenarios it is shown between brackets behind the substance name. Selecting such a substance will result in a project that cannot be exported to the other models.

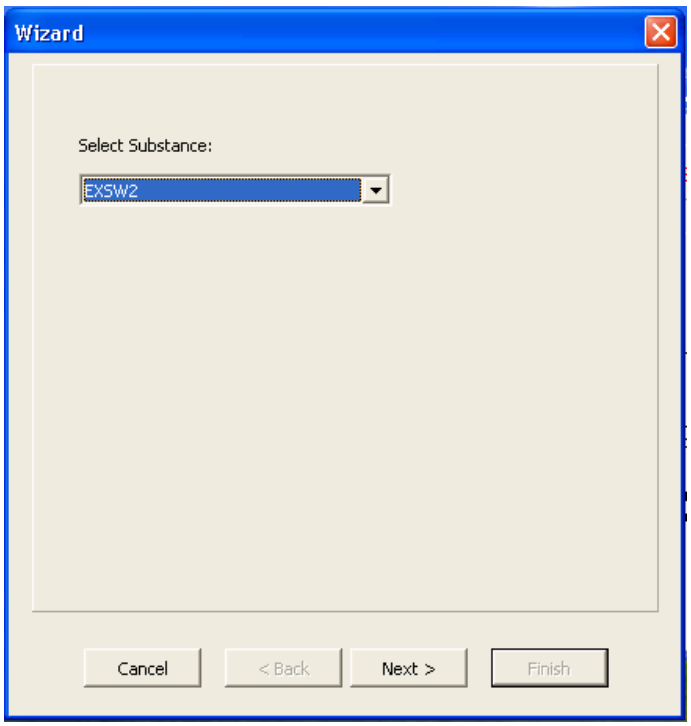

Figure 2.6. The User-Defined Wizard – Substance.

After selecting the substance, the user has to click on the 'Next' button. Then the form presented in Figure 2.7 is shown on the screen. In the example, the user has selected four crops: spring oil seed rape, maize, legumes and grass/alfalfa. The user can add or delete crops from the list by clicking on the '>' button or the '<' button. It is also possible to put all crops in the list of selected crops by clicking on '>>'. Removing all crops from the list of selected crops can be done by clicking on '<<'.

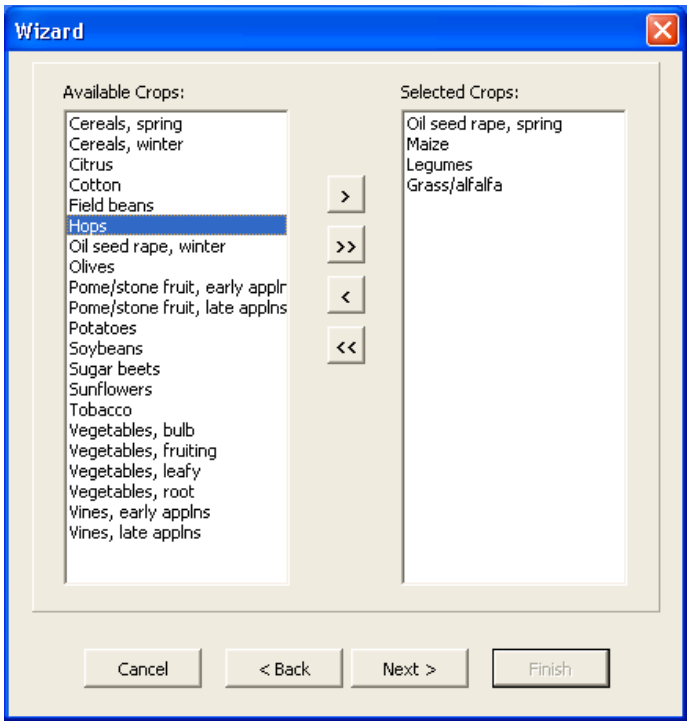

Figure 2.7. The User-Defined Wizard – Crops.

After the crops have been selected, the user continues the wizard procedure by clicking on 'Next'. Then the form with the possible water body types is shown on the screen (Figure 2.8). On this form the user can specify for which water body types runs need to be created. The user can select or deselect a water body type by marking the check boxes on the left of the water body type names.

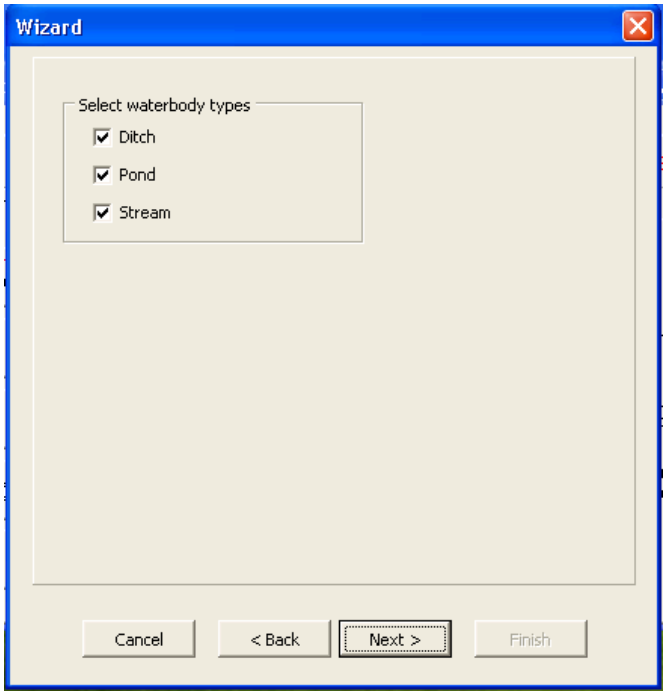

Figure 2.8. The User-Defined Wizard – Water bodies.

After the selection of the water body types the user continues by clicking on 'Next'. The next wizard form shows the list of available FOCUS Surface Water Scenarios. Only scenarios for which the crop – water body type combinations have been defined are included in this list. In the example shown in Figure 2.9, the scenarios D3, D4, and R1 are selected. The user can add or delete scenarios from the list by clicking on the '>' button or the '<' button. The user can select all or deselect all scenarios by clicking on '>>' or '<<', respectively.

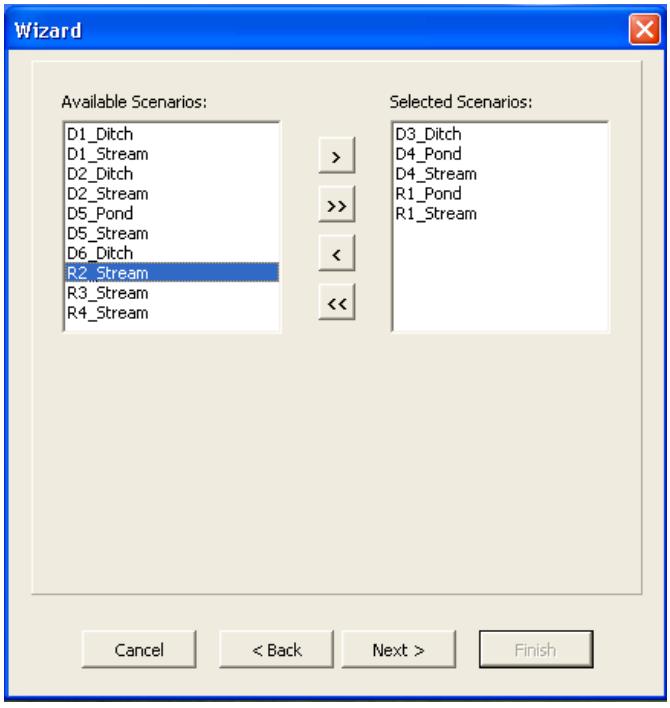

Figure 2.9. The User-Defined Wizard – Scenarios

After the selection of the scenarios of interest, the user continues by clicking on 'Next'. Then the last form of the wizard is shown on the screen (Figure 2.10). On this form the user has to specify the name and the description of the project. Using the User-Defined wizard, the project name is set by default to [project_SubstanceName], but this can be modified by the user.

All SWASH output is put the subdirectory C:\SwashProjects. The SWASH output path can be changed by clicking on the button on the right-hand side of the 'path' field. The directory for the output of a SWASH project is set to C:\SwashProjects\[project_name]. For the example shown in this section the path is C:\SwashProjects\FOCUS_Test_2. The output for PRZM, MACRO and TOXSWA are put into subdirectories \MACRO, \PRZM and \TOXSWA, respectively.

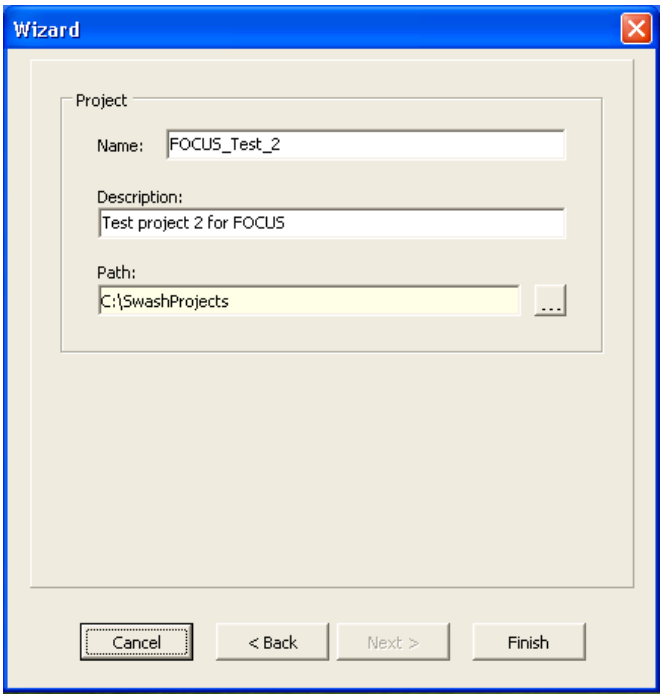

Figure 2.10. The User-Defined Wizard – Project Name and description

After clicking on 'Finish' the runs are generated and the user gets a message on the number of runs created. After clicking on 'OK' the user returns to the main window of SWASH.

2.1.5 View Projects and Define Applications

After clicking on the button 'View Projects and Define Applications' on the main window, the form shown in Figure 2.4 is displayed on the screen (the example project from Section 2.1.3). The 'Overview of composed projects' form consist of two parts:

- The upper part is a browse part, where the user can browse through the list of available projects. For each project there are several columns indicating: the project ID, the description, created and modified dates, the path and the status.
  The status can be 'OK' when a project can be run, or 'not OK' when a project cannot be run (e.g. when a substance is 'ambiguous' and/or 'incomplete'.

- In the lower part all the runs within the selected project are shown. For each run there are several columns indicating: the run ID, the caption, the substance, the crop, the number of season (the first or the second crop in the season), the location, the water layer, the number of applications, and selected for report.

By default all runs are selected for report ('True'), which means that the characteristics of each run can be exported to PRZM, MACRO and TOXSWA. If the user wants to select only some runs to be exported, than he can double click on 'True' and select the option 'False'. The user can also select or unselect all runs for the report by clicking on the checkbox 'Select/Unselect all Runs' at the top right corner of the 'Runs' section of the 'Overview' form.

In Figure 2.4 the runs created by the User-Defined FOCUS wizard is shown. If more runs have been created that the window can show, the other runs can be seen using the scroll bar on the right hand-side of the 'Runs' section of the 'Overview' window.

Useful functionalities on the 'Overview of composed projects' window are the buttons:

- 'Export FOCUS input to MACRO, PRZM and TOXSWA', which allows the user to export a project to PRZM, MACRO and TOXSWA and therefore to run the models.
- 'View Report', clicking on this button an overview report is composed by SWASH, which lists all the FOCUS runs the user needs to do. It is useful to print this report to keep track of the runs to be done in the various model shells. An example of this report is given in Annex 2.
- 'Copy project', which allows the user to copy the selected project. The user can only edit the project name and description.
- 'Remove run', which allows the user to delete a selected run in a selected project. Note that a deleted runID number will not be used again in the SWASH database.

After clicking on the button 'View and Edit Applications' on the 'Overview of composed projects' window, the form shown in Figure 2.5 is displayed on the screen.

On this form the scenario, crop, number of crop in season and water body type for each run are fixed and are highlighted in yellow. The user can edit the application input data for the FOCUS runs:

- The application method: first select a run then click on the cell in the 'Application method' column for this run: a list of available options is shown.
- The number of applications.
- The first possible day of application (entered as day-in-year number; SWASH converts this in day-month value).
- The last possible day of application (entered as day-in-year number; SWASH converts this in day-month value).
- The minimum time interval (in days) between two consecutive applications.

A Day-In-Year calendar is included in Annex 3. This can help the user to find quickly the day-in-year number for the first and last possible days of application.

Before increasing the number of applications, the user has to widen the time window between the first possible day of application and the last possible day of application. The minimum time window that can be used is given by the following equation (FOCUS, 2001):

$$\text{Window} = 30 + (n-1) \cdot \text{int} \qquad \text{(eq 1)}$$

In which:

n = number of applications;

int = minimum interval between two consecutive applications (days).

Default values used by SWASH are two weeks before emergence of the crop for the first possible day of application and 16 days after emergence of the crop for the last possible day of application. Thus, the period between the first and last possible day of a single application is 30 days.

If the number of applications is changed for a scenario with more than one water body type then the new number of applications is set for all water body types in that scenario.

The input data on the application in the box in the lower-left part of the 'Applications' form, as shown in Figure 2.11 are input for a FOCUS run with a drainage scenario. If the dosage is different from the default value of 1 kg ha^{-1}, then the user has to specify the dosage (in kg ha^{-1}) for each run.

Upon selection of a FOCUS run with a run-off scenario, the user has to enter a few more data to complete the run information, because the PRZM model has more options for the method of application (Figure 2.12). Here the Chemical Application Method (CAM) types in PRZM are briefly described:

1. Application to soil with linear decline to user-specified depth.
2. Application to foliage with interception based on crop canopy and linear decline in soil to user-specified depth.
3. Not used in FOCUS Step 3.
4. Incorporation in soil with uniform profile and user-specified depth.

5. Incorporation in soil with profile linearly increasing to user-specified depth.
6. Incorporation in soil with profile linearly decreasing to user-specified depth.
7. Not used in FOCUS Step 3.
8. Incorporation in soil with total application located at user-specified depth.

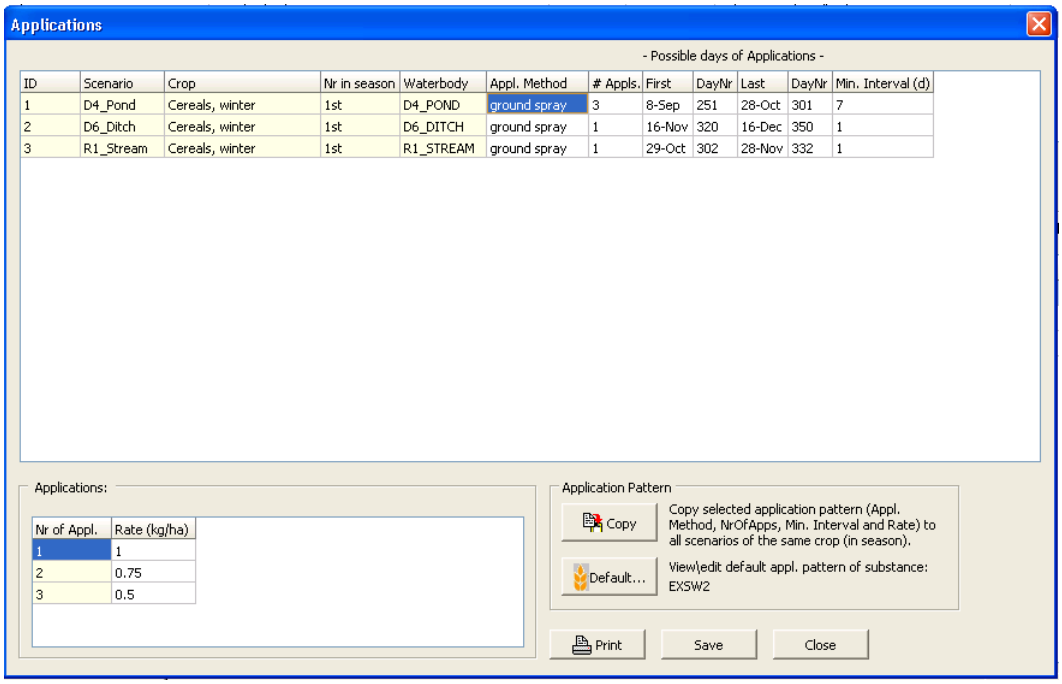

Figure 2.11. Application data for the runs in a project; a run for a Drainage scenario is selected.

Therefore, the user has to specify the method of application and the incorporated depth (Figure 2.12).

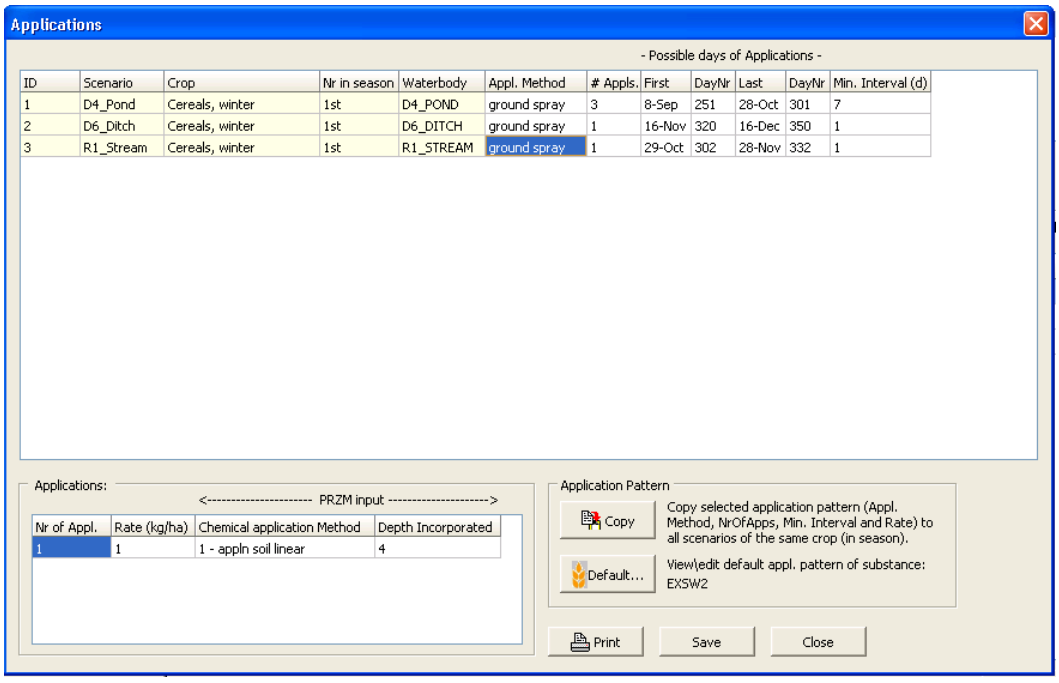

Figure 2.12. Application data for the runs in a project; a run for a Run-off scenario is selected.

The overview of the application data for runs in the project can be printed by clicking on the 'Print' button.

The user has to be aware that the scenarios of a location are linked. For example if the application rate in the D1_Ditch scenario is changed also the rate in the D1_Stream will change into the entered value.

The 'Copy' button in the 'Application pattern' section allows the user to copy the application method, the number of applications, the application rates and the minimum interval between two consecutive applications to all runs in the same project. Please note that the period between the first and last possible days should be wide enough to allow the application pattern to be copied. If this is not the case, SWASH will give a message that the time window is not large enough and should be adjusted.

The application pattern defines the method, time period, minimum time interval, number of applications and the rates. From these data the Pesticide Application Timer (PAT, see FOCUS, 2001) determines the exact dates of application using a standard procedure. PAT has been included in the MACRO and PRZM models to minimise the influence of the user to choose the application date, as both surface run-off and subsurface macropore flow are 'event-driven' and strongly depend on the rainfall pattern immediately after application.

For applications in vines or pome/stone fruit, a differentiation between early and late applications is made. This distinction in the Ganzelmeier dataset (Ganzelmeier *et al*., 1995) is made because of the different drift levels at early and late growth stages for these crops and because there are plant protection products which are only used either in early or in late growth stages.

On the 'Applications' window, the user can enter application patterns for a substance, that differ from the default that SWASH defines. The form with data on the default applications is shown in Figure 2.13 and is opened by clicking on the button 'Default' in the 'Applications' window.

The name of the substance the user has selected is displayed in the field at the top of the form. First, the user has to add an entry by clicking on 'add'. Next the user has to set the cursor on the field of this entry in crop column, click again on this field to edit and then once more to obtain the crop list from which the user can select one. For the other fields of the new entry, the user has to follow the same procedure as for the 'crop' column. The fields that contain numbers (e.g. # Appls, DayNr) can be edited by setting the cursor on the field to be edited. Note that the dates in the date columns are adjusted automatically to the values entered for the day-in-year numbers.

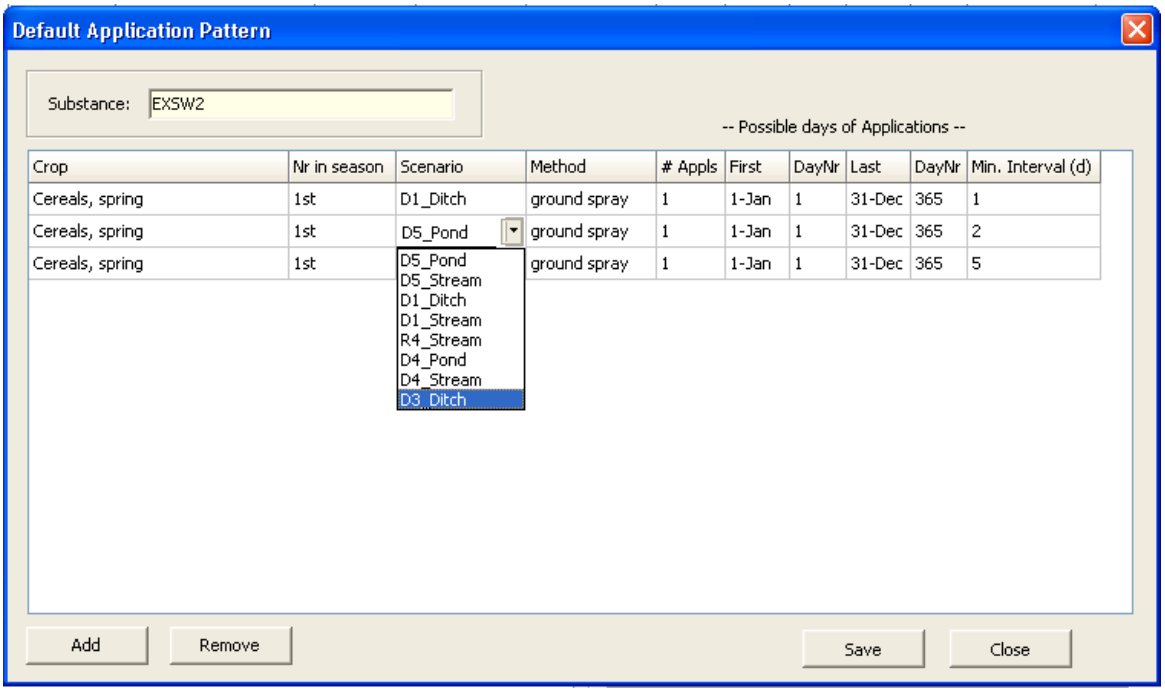

Figure 2.13. The application form of SWASH – The default application pattern.

The user gets a warning if the application is outside the period of 14 days before start of the cropping period and the end of the cropping period. If the period between the first day-in-year and the last day-in-year for the application is outside the cropping period, the pesticide is applied to bare soil.

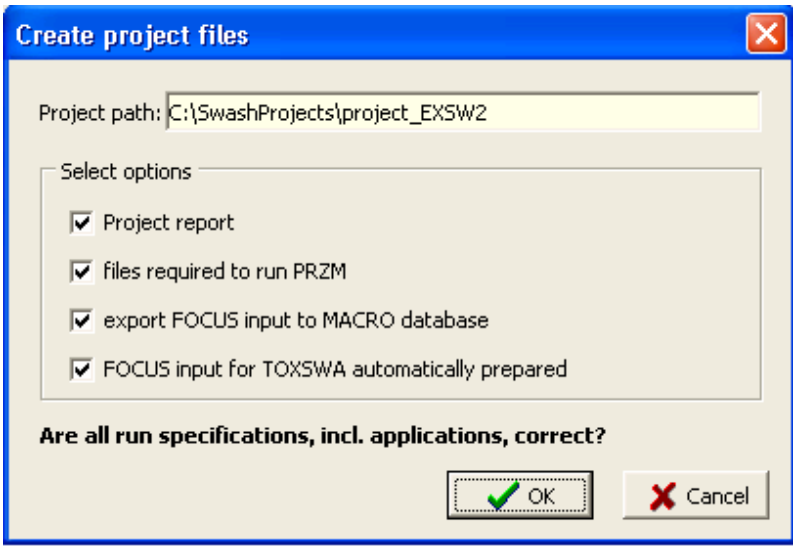

Figure 2.14. Create project files – options.

Once all input data have been entered correctly, the user returns to the 'Overview of composed projects' window by clicking on 'OK'. Now the user can click on the button 'Export FOCUS input to MACRO, PRZM and TOXSWA' to prepare the input for the runs for MACRO, PRZM and TOXSWA. There are two possibilities:

1. The project contains single application runs with spray drift, or multiple application runs without spray drift. Then, the 'Create project files' form is shown directly (Figure 2.14).
2. The project contains multiple application runs with spray drift (ground blast, air blast or aerial). Then, the user is asked if the project should be copied for a single application assessment (see also Section 3.2) as shown in Figure 2.15. How the runs in the project are copied to a single application assessment is indicated in the form shown in Figure 2.16. Thereafter, the 'Create project files' form is shown.

The options on the 'Create project files' form are shown in Figure 2.14. The user can select one or more options. After the appropriate options have been selected the user clicks on 'OK'.

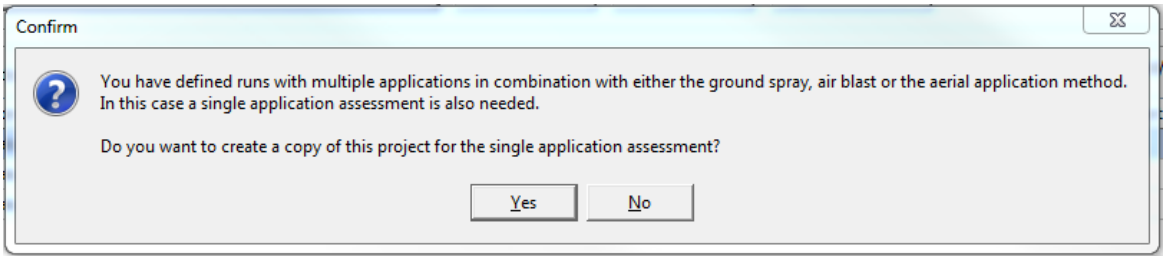

Figure 2.15. Option to copy project for single application assessment.

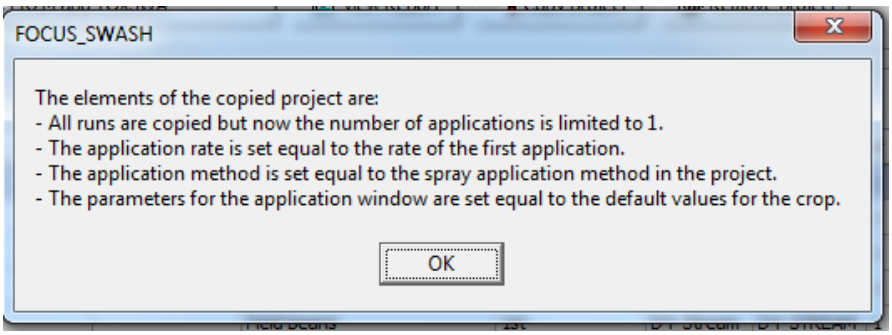

Figure 2.16. Informative view after selecting copy project for single application assessment.

Now all input data have been prepared to run the individual FOCUS models MACRO, PRZM and TOXSWA. The user can start these runs by going to the main window of SWASH and click on the PRZM or the MACRO button to start up the PRZM or the MACRO shell and select and execute the runs required. These runs must be executed first to create the m2t and p2t files before TOXSWA can be

run. Note that it is not possible to run FOCUS surface water models concurrently in SWASH. Its strongly recommended to start runs for all FOCUS models via SWASH to obtain consistent runs for the consecutive model calculations.

2.1.6 Metabolites

Besides parent compounds also metabolites can be simulated by the FOCUS surface water models. MACRO and PRZM simulate soil metabolites. These metabolites can enter the water body, where their fate is simulated by TOXSWA. The new version of TOXSWA (FOCUS_TOXSWA_4.4.3) allows to simulate the fate of metabolites formed in water and sediment.

MACRO and PRZM can simulate the following metabolite schemes for the soil metabolites:

1. parent → metabolite A1
2. parent → metabolite A1
   → metabolite B1

Additionally PRZM can simulate also the metabolite scheme:

3. parent → metabolite A1 → metabolite A2.

To add a metabolite to a parent compound, the user first needs to add the metabolite substance in SPIN. All the required parameters of the metabolite substance have to be set. Thereafter the parent substance to which the metabolite belongs has to be selected. Then the metabolite form table has to be opened by clicking on the open metabolites form  button on the right hand side of the main window. The user has to choose the appropriate compartment table (soil, surface water, sediment) and then the metabolite can be added using the  button. Now the user can select the metabolite from the drop-down menu. Thereafter the fraction of metabolite formed from the parent in the compartment can be entered. The same procedure has to be followed in case a subsequent metabolite has to be linked to a first metabolite.

There are some cases in which the parents and/or the metabolites will appear in SWASH as 'ambiguous', i.e. the metabolite scheme cannot be handled by either MACRO or PRZM:

1. parent → metabolite A1
   → metabolite B1
   → metabolite C1

2. parent → metabolite A1→ metabolite A2
   → metabolite B1

3. parent → metabolite A1→ metabolite A2
   → metabolite A3

4. parentX → metabolite A1
   parentY → metabolite A1

When a substance is shown as 'ambiguous', the data are not transferred to MACRO and/or PRZM. It is however possible to create a project, but it is not possible to run that project. Note that the warning of ambiguity of the substance is shown when the user selects the substance in a project, and not during the preparation of the substances in SPIN.

In case a parent compound has the following scheme:

parent → metabolite A1→ metabolite A2 → metabolite A3

the substances will not appear as 'ambiguous', but the user should be aware that metabolite A3 will not be simulated by either MACRO or PRZM (however metabolite A1 will be simulate by both MACRO and PRZM, while metabolite A2 will be simulated only by PRZM).

TOXSWA simulates metabolites formed in water and in sediment. In stream scenarios parents enter the upstream catchment of the stream via spray drift and/or via drainage/runoff. For primary metabolites formed in water formation of the metabolite in the upstream catchment is accounted for (Adriaanse *et al*., 2014). The metabolite mass formed in the upstream catchment is calculated using a correction factor for metabolite formation ($CF_{m,,up}$). This correction factor is substance specific and scenario specific (Adriaanse *et al.*, 2014).

In FOCUS_SWASH 5.3 the calculation of the correction factor $CF_{m,,up}$ is automated. When the parent substance has one or more primary water metabolites the correction factor is calculated and stored in the database for each primary water metabolite. The procedure of the calculation is given in Appendix 2 of Adriaanse *et al*. (2014). The calculated values can be viewed in the TOXSWA GUI at the Entries tab of the Edit runs form (see Annex 4).

2.1.7 Running MACRO

After exporting the data of a project to the MACRO database, the user can start the MACRO shell by clicking on the 'MACRO' button on the main window of SWASH. In this section a short introduction on running the FOCUS MACRO model is given. A more detailed description is given in FOCUS (2001, Appendix J), version 2 of the parameterisation document. The parameterisation of drainage scenarios, described in Appendix C of FOCUS, 2001, was updated. A document is available on the FOCUS website (http://focus.jrc.ec.europa.eu/sw/index.html), describing the changes in the parameterisation of FOCUS_MACRO_5.5.3. The updates were incorporated in the new version of MACRO in FOCUS.

The main window of the MACRO in FOCUS shell is shown in Figure 2.17.

To perform a run of the project the following steps have to be done:
- Select from the Menu bar at the top of the MACRO main window 'Define scenario' and then select 'Surface Water' (Figure 2.17).
- The 'FOCUS scenario' window appears now on the screen (Figure 2.18).
- Then select the crop for the run to be executed using the pull-down menu showing the crop list.
- Select the drainage scenario for the run to be executed using the pull-down menu showing the valid scenarios for the crop selected.

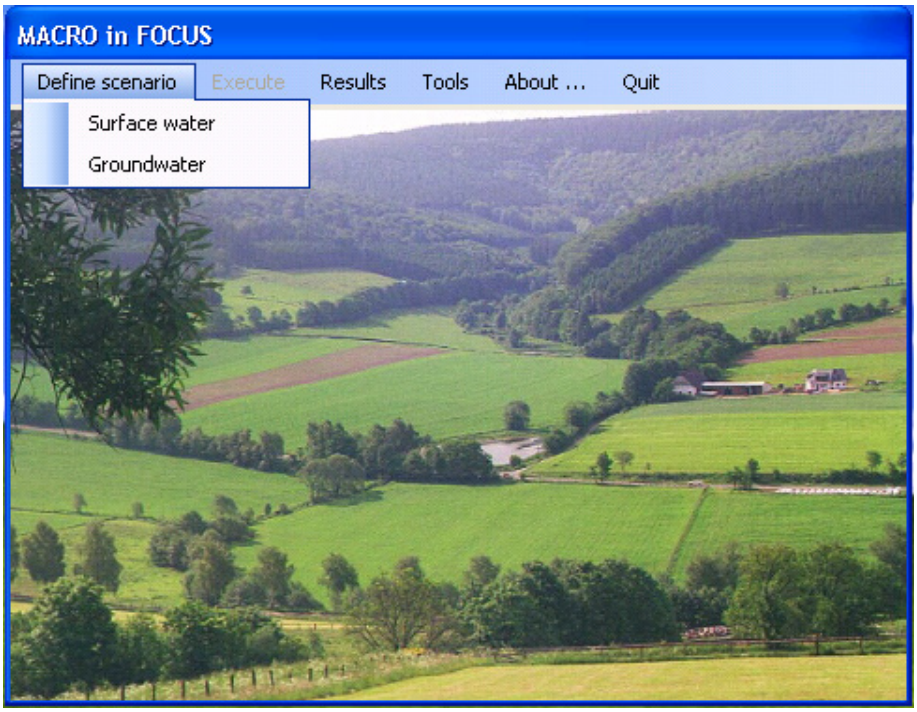

Figure 2.17. Main window of MACRO in FOCUS.

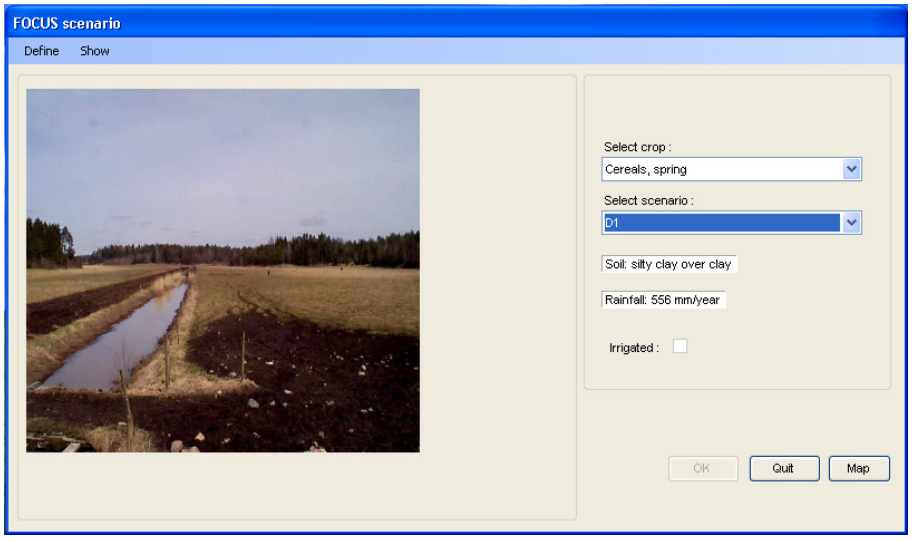

Figure 2.18. 'FOCUS scenario' window in MACRO.

Select from the Menu bar at the top of the 'FOCUS scenario' window 'Define' and then select 'parent compound'. The substance form is now shown (Figure 2.19).

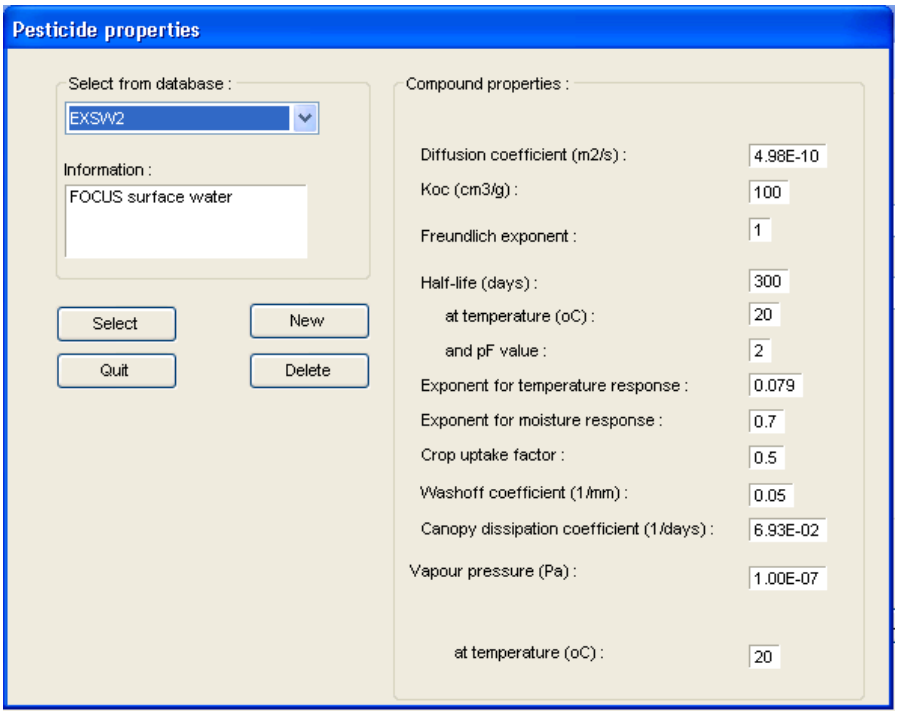

Figure 2.19. Substance form of MACRO in FOCUS.

- Select the substance for the run to be executed from the list of substances using the pull-down menu and confirm this by clicking on the button 'Select'.
- Select from the Menu bar at the top of the 'FOCUS scenario' window 'Define' and select 'Applications'. Now the form presented in Figure 2.20 will be shown.
- Select the runID for the run to be executed; this runID is the same as the runID of the corresponding run in SWASH. Next click on the button 'OK'. The application input data have been transferred from SWASH to MACRO.
- When a parent compound has a metabolite select from the Menu bar at the top of the 'FOCUS scenario' window 'Define' and then select 'metabolite'. The substance form is now shown. Select the substance for the run to be executed from the list of substances using the pull-down menu and confirm this by clicking on the button 'Select'.
- The 'FOCUS scenario' window will appear on the screen (Figure 2.18). Click on the button 'OK'. The MACRO run is now fully defined and the main window of the MACRO is shown (Figure 2.17).

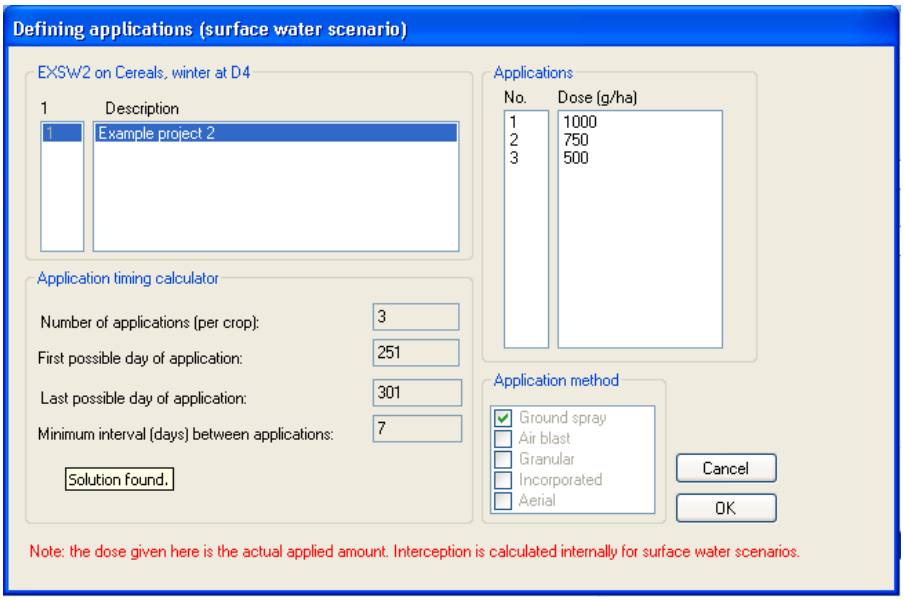

Figure 2.20. Application form of MACRO in FOCUS.

- In the Menu bar of the MACRO main window (Figure 2.17) select 'Execute'. Note that the user can choose whether to run the current run by selecting 'current run' or set up a batch file (see FOCUS, 2001 – Appendix J for more details). Then the MACRO run will now start.
- After completion of the simulation run, the .m2t output file has to be created. This file contains the TOXSWA input data on the drainage and the pesticide fluxes that enter the surface water.
- The m2t file can be created by selecting 'Results' in the menu bar of the main window of MACRO. Now the form presented in Figure 2.21 will be shown.

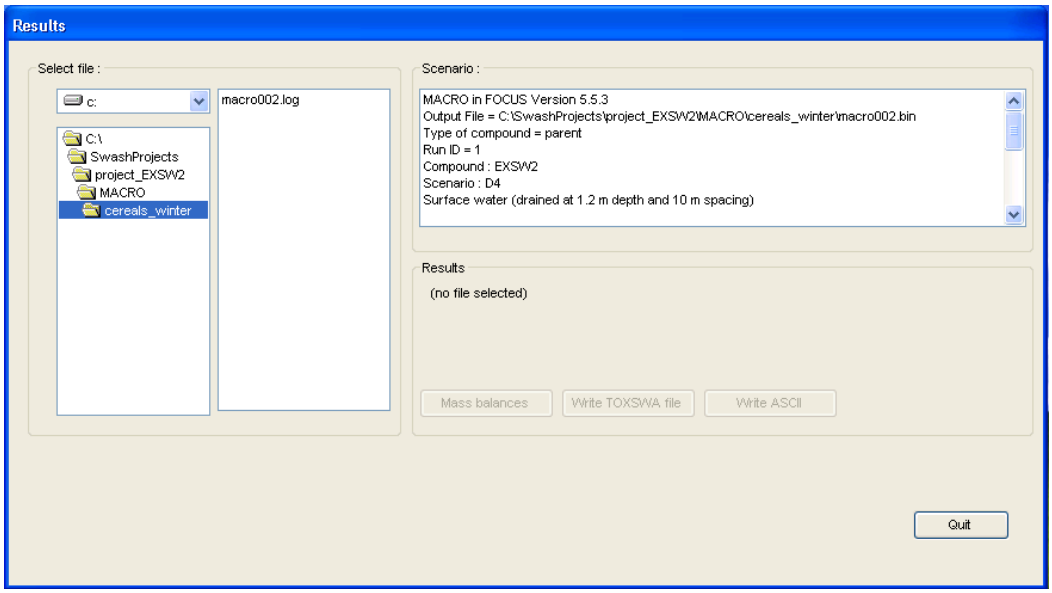

Figure 2.21. Creation of the MACRO output file with input to be read by TOXSWA.

The following steps have to be performed:

- Select the log file corresponding to the run completed; the specifications of the run, e.g. the substance, the scenario, the crop and the runID are listed in the text box in the 'scenario' section of the form.
- Click on 'write TOXSWA file' and MACRO starts to process the output data to create the m2t file that contains the input for TOXSWA. Once the m2t file has been created MACRO writes a message to the screen specifying the directory where this file has been put as well as the file name. Click on OK to return to the main window of MACRO.
- If a parent compound has metabolites, m2t files have to be created also for each metabolite following the same procedure stated above for the parent compound. Log files corresponding to the run done for the metabolite will be shown.

Note that in case a parent compound has two metabolites (hence same SWASH run ID), two runs for the parent compound will be carried out, one for each metabolite. Use the 'write TOXSWA file' twice for the first metabolite. Then, the second time, the name of the m2t file for the metabolite, e.g. macro0001_m.m2t, will be changed into macro0001_m_1.m2t (if a second m2t file for the second metabolite is to be created). Using 'write TOXSWA file' for the second m2t file (second metabolite) the resulting file will be named macro0001_m_2.m2t.

2.1.8 Running PRZM

The user can start the PRZM shell by clicking on the 'PRZM' button on the main window of SWASH. In this section a short introduction on running the FOCUS PRZM model is given. A description of PRZM input parameters, PRZM input and output files is given in FOCUS (2001, Appendix K), but no guidance is given on how to run the model. The main window of the PRZM shell is shown in Figure 2.22.

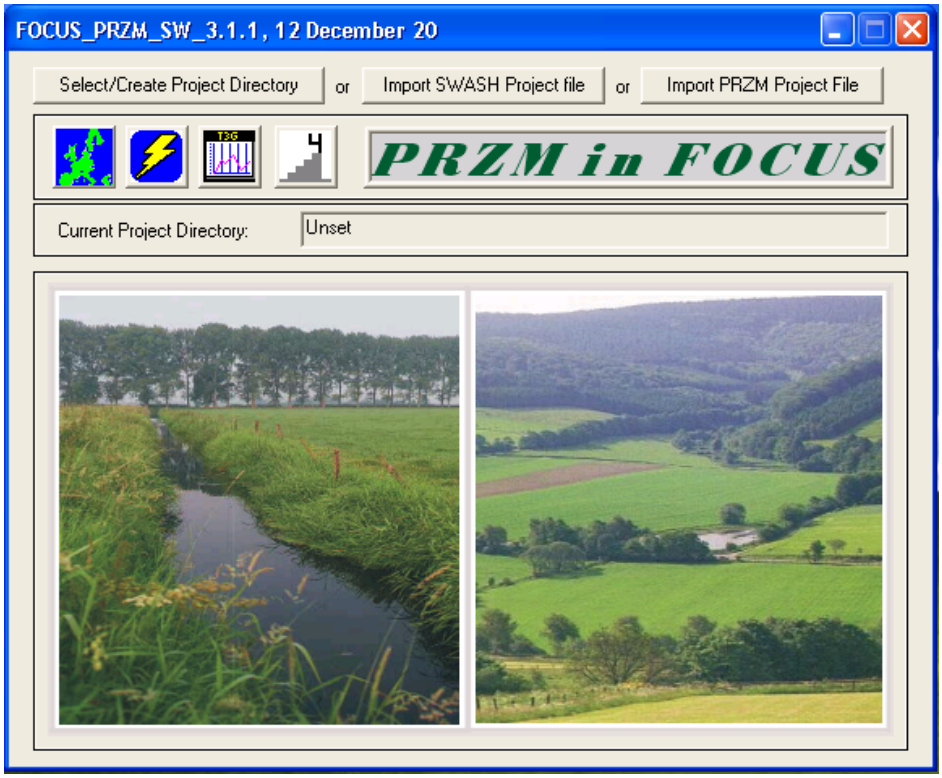

Figure 2.22. Main window of FOCUS_PRZM.

To start a FOCUS surface water run in PRZM the following steps have to be done:

- Click on the button 'Import SWASH Project File'.
- Now the PRZM window for selecting a SWASH projects will be shown (Figure 2.23).
- Select the project containing the run(s) to be executed.
- Select the crop from the list of crops in the project. It should be noted that a SWASH project created with the User-defined Wizard may contain multiple crops.
- Select 'Perform Step 3 calculation' (default option in PRZM).
- Click on 'OK'.
- Select 'Write' from the Menu bar and PRZM gives the message 'Output files successfully written'; click on 'OK and exit'.
- Click on the button with the thunderbolt (See Figure 2.22).
- Now the PRZM run(s) will be started.
- The PRZM model automatically prepares p2t files with run-off and erosion fluxes for input in TOXSWA.

PRZM can describe three types of transformation schemes with up to two metabolites: 1) a parent with one metabolite, 2) a parent with two metabolites and 3) a parent with two sequential metabolites. In case metabolites are simulated, these will be automatically run and p2t files will be created as well.

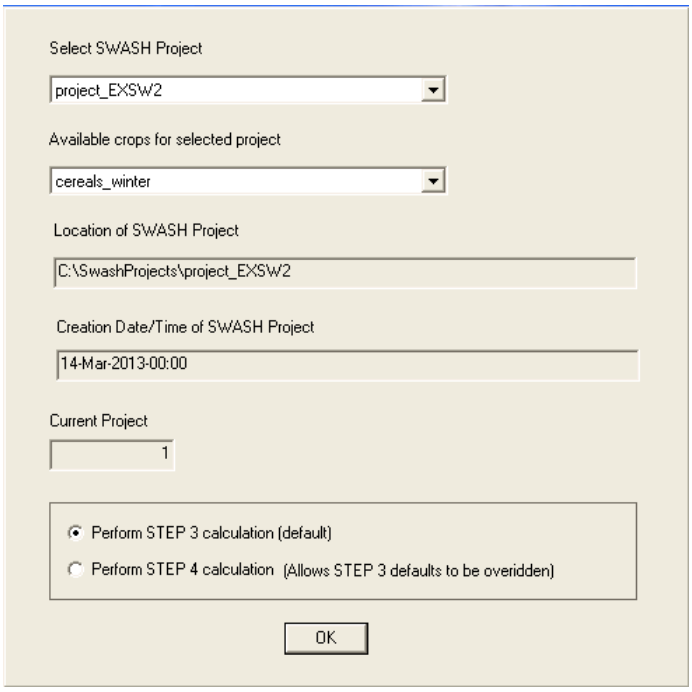

Figure 2.23. SWASH Project window of FOCUS_PRZM.

2.1.9 Running TOXSWA

The user can start the TOXSWA shell by clicking on the 'TOXSWA' button on the main window of SWASH. The main window of the TOXSWA user interface is shown in Figure 2.24. The User's Manual for FOCUS TOXSWA is available (Beltman *et al*., 2014). In the following section only a short description on running FOCUS_TOXSWA_4.4.3 is given.

The TOXSWA user interface extracts all information from the same database as SWASH, so there is no separate data exchange needed as is necessary for PRZM and MACRO.

In order to run TOXSWA the following steps have to be done:

- Select the project containing the runs to be executed (Figure 2.24).
- and click on 'Open selected project'.

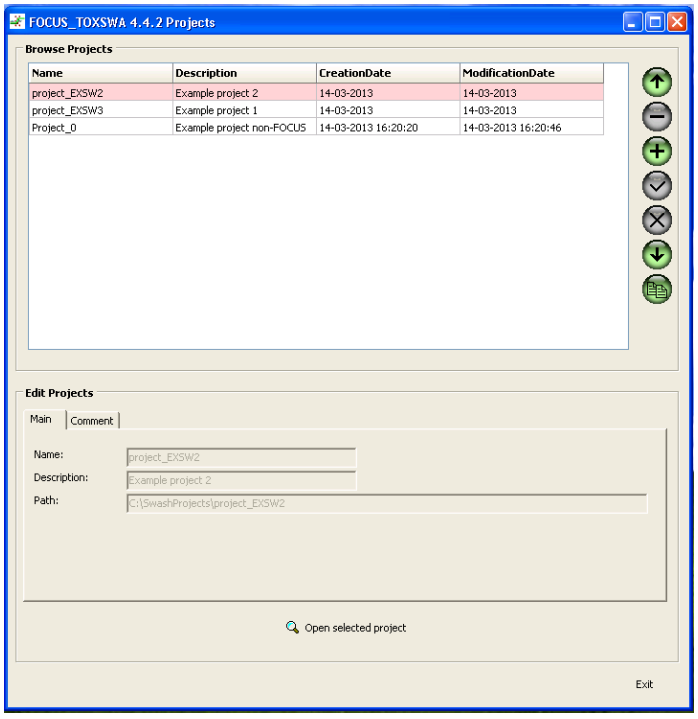

Figure 2.24. Project window of FOCUS_TOXSWA.

- On the TOXSWA main window (Figure 2.25) all the runs included in the project are listed in the 'Browse run' tab. On the 'Edit run' tab all the details for each run are shown. Runs created via SWASH cannot be modified.

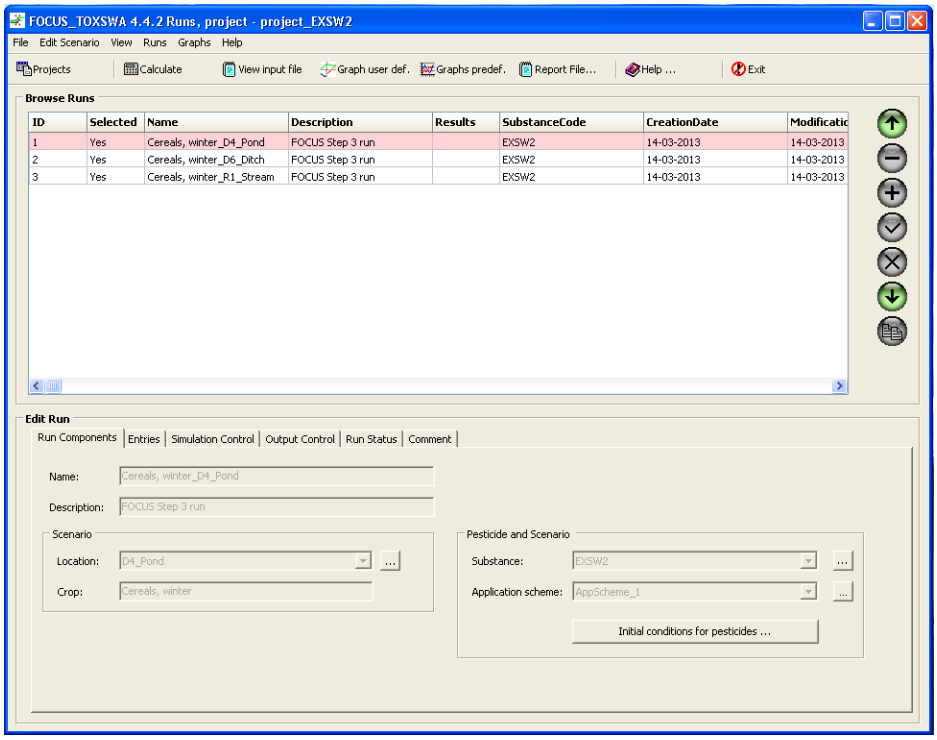

Figure2.25. Project window of FOCUS_TOXSWA.

- All the runs selected in SWASH for being exported in TOXSWA are selected for being executed in TOXSWA. If the user wants to deselect some runs he/she can double click on 'Yes' in the column selected. Otherwise, for selecting or deselecting all runs at once the user can click on 'Runs' in the menu bar and choose 'select all runs' or 'deselect all runs'.
- Click on the button 'Calculate'. Now the runs selected will be executed one after another.
- Clicking on 'View' on the main bar (Figure 2.26), the user can see the input file, the report file, the summary file, the log file and the error file.

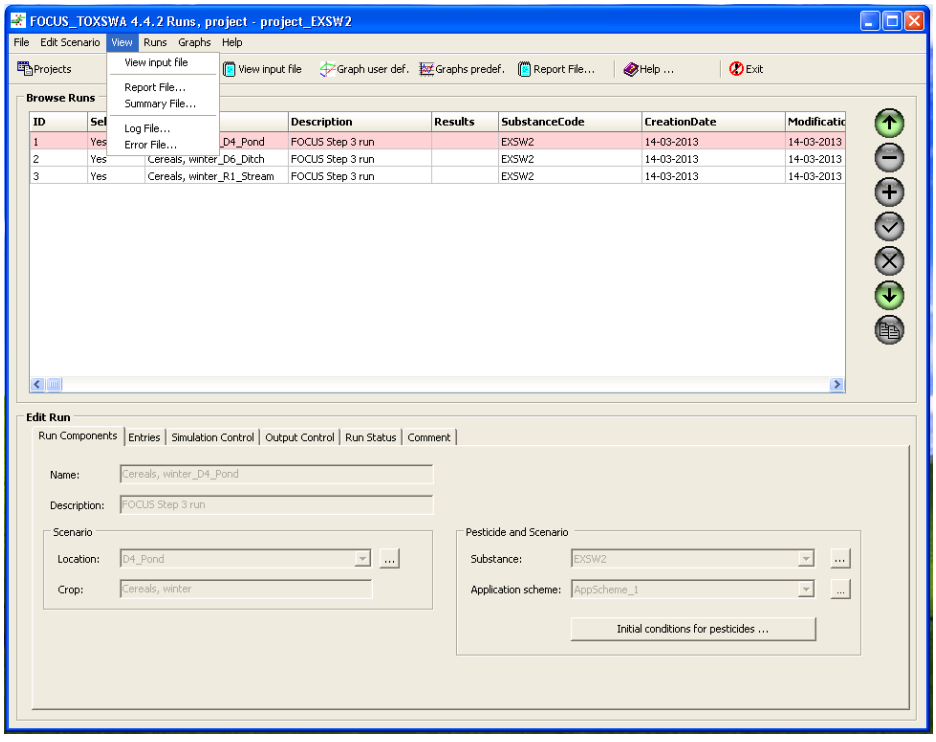

Figure 2.26. 'View' menu on the project window of FOCUS_TOXSWA.

- Clicking on the button 'Report file' the user can obtain a report summarizing the target data for the exposure assessment for each run executed.
- Clicking on 'View input file' the TOXSWA input file will be shown.

2.2 The Main Window - Information

As stated above the main window of SWASH consists of two parts, 'Actions' and 'Information'. The first part, 'Actions', has been described in Section 2.1, the second part, 'Information' is described in this section. It is displayed after clicking on the 'Information' tab and the content of this tab is shown in Figure 2.27. In the 'Information' part the user is only informed about certain aspects of Step 3 exposure assessment, but no actions are executed, e.g. no changes take place in the database, no input is prepared, no projects are created and no drift deposition values are transferred to TOXSWA as input.

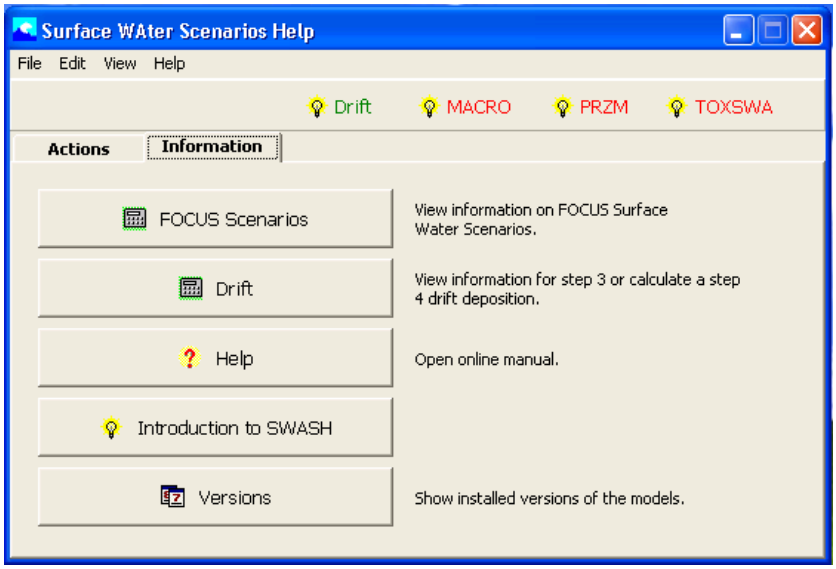

Figure 2.27. The main window of the SWASH interface with the 'Information' tab displayed.

The 'Information' page of the main window of SWASH contains five buttons. The function of the buttons will be briefly described here, but more details about the FOCUS Scenarios and Drift is given in Sections 2.2.1 and 2.2.2 respectively. The button 'FOCUS Scenarios' gives the user access to information on the FOCUS Surface Water Scenarios, e.g. the list of relevant crops for each scenario. Maps are available too to give the user an indication on the extent of occurrence of a scenario within the European Union (in 2003, so before accession of the new member states in 2004).

The 'Drift' button will lead the user to the FOCUS Drift Calculator. This is a tool to calculate the drift percentage and areic deposition as a function of water body characteristics and application method.

The 'Help' button gives of access to the pdf of the present user manual.

Behind the 'Introduction to SWASH' button an outline is presented of the main functions of SWASH and the use of the wizards to compose projects, consisting of FOCUS surface water runs. Furthermore, a brief explanation on how running the separate models (MACRO, PRZM and TOXSWA) with the aid of their own shells is provided.

The 'Versions' button gives information on the FOCUS version numbers of the different models – PRZM, MACRO and TOXSWA – that are integrated in SWASH as well as the Drift Calculator. The version number contains a number for each component in the software package, i.e. model-shell-database numbers. If the model and shell are integrated, then only one number is given for the shell-model combination.

2.2.1 FOCUS scenarios

The use of the button 'FOCUS scenarios' results in a display of information about the crops, scenario types and water body types as identified by the FOCUS Working Group on Surface Water Scenarios. After clicking on this button, the 'FOCUS scenarios' page window presented in Figure 2.28 is shown on the screen. On this page three tabs with information are available. On the 'Crops' tab (Figure 2.28) the full crop list is shown in the upper part of the form. Using the scroll bar, the user can select one of the crops and the scenarios where this crop occurs are listed in the lower part of the form, as well as the emergence and harvest dates for each scenario.

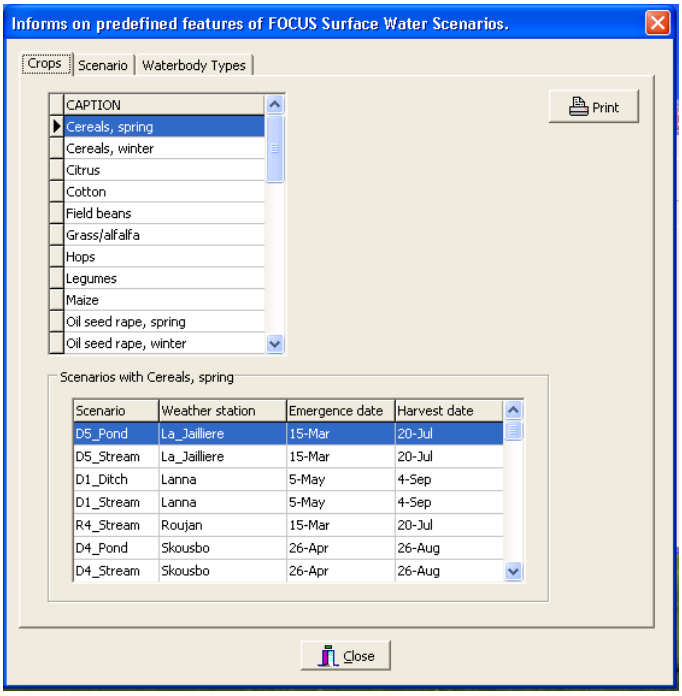

Figure 2.28. FOCUS Surface Water Scenarios – Crops.

On the 'Scenario' tab, as shown in Figure 2.29, the complete list of available scenarios is presented in the box on the left. Upon selection of one of the scenarios, the available crops for that scenario are shown in the box on the right. After clicking on the 'Map' button, a map of the European Union is displayed on the screen, in which the occurrence of the selected scenario is indicated.

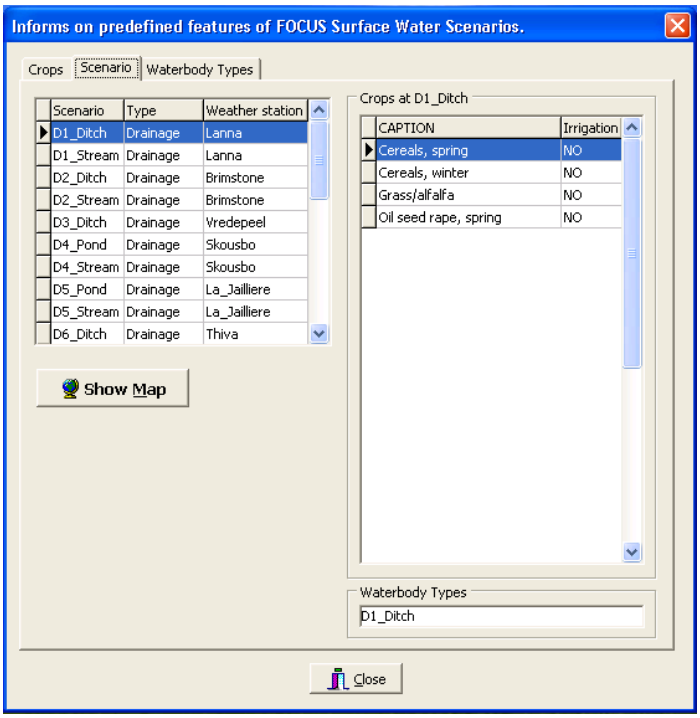

Figure 2.29. FOCUS Surface Water Scenarios – Scenario Types.

On the 'Water Body Types' tab, as shown in Figure 2.30, the user can get a list of available scenarios for a specific water body type. In the example presented in Figure 2.30, the 'Ditch' Water Body Type is selected. In the set of FOCUS scenarios there are only four available scenarios (all drainage) for the FOCUS Ditch.

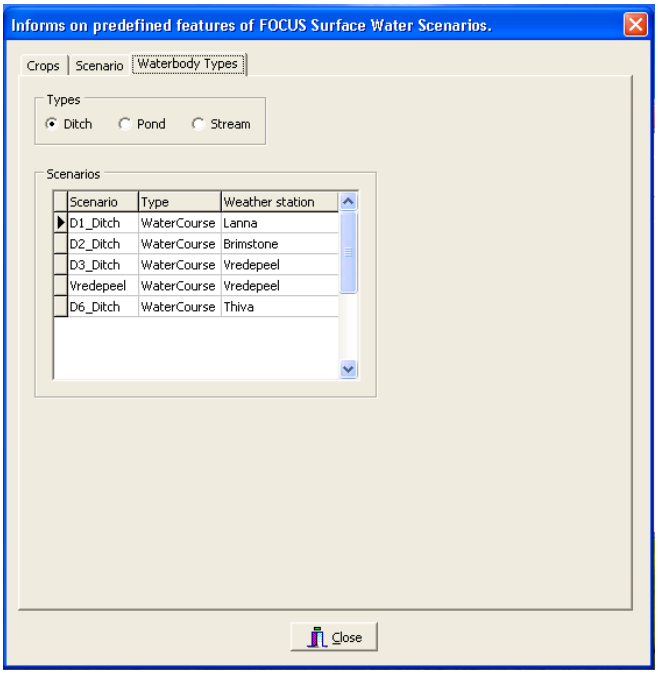

Figure 2.30. FOCUS Surface Water Scenarios – Water Body Types.

2.2.2 Drift

The 'Drift' button has been added on the 'Information' tab to inform the user about the calculation of the deposition due to spray drift in the FOCUS scenarios. After clicking on the 'Drift' button, the form shown in Figure 2.31 is shown on the screen. The user has to enter values in the 'Input' section of the form. First, the dosage has to be specified in g ha^{-1}. Next the crop has to be selected using the pull-down menu for the crop. In the example shown, spring cereals is selected. Then the water body type has to be specified. For FOCUS Step 3, 'FOCUS values' should be selected in the field on the right of the line 'Use FOCUS (Step 3) or mitigation distances (m)?'

The underlying drift data are those presented by BBA (2000). The BBA data comprise the data obtained from field experiments described by Ganzelmeier (1995) and those from field experiments carried out between 1996 and 1999 by Rautmann *et al*. (2001). The data for aerial applications have been obtained from experiments described by SDTF (1999). The numbers shown on the window with a blue background are for information purposes only. These data refer to the dimensions of the water body and the field site, and the regression parameters used in the drift calculations.

The output on the drift percentage for the application conditions specified as well as the mass loading on the receiving water body are shown in the lower two sections of the 'Drift' form. These numbers are shown in fields with a yellow background. . For Step 3 calculations the results of the Drift calculator are for information purposes only, since SWASH transfers these data automatically to TOXSWA.

On the bottom right corner of the 'Drift' form, the button 'Save Screen' can be used to save the information displayed as a bitmap and the button 'Print' to print the window. After clicking on 'Close' the user returns to the main window of SWASH.

It should be noted that when the number of applications increases, the deposition for each individual spray event decreases. This is due to the fact that the 90th percentile as calculated by the FOCUS Drift Calculator is based on the over-all probability of occurrence, but the probability of occurrence of one spray event in a series of applications can decrease to the 67-percentile with corresponding lower depositions. Therefore, it is recommended to perform always a risk assessment for a single application (see Section 3.2).

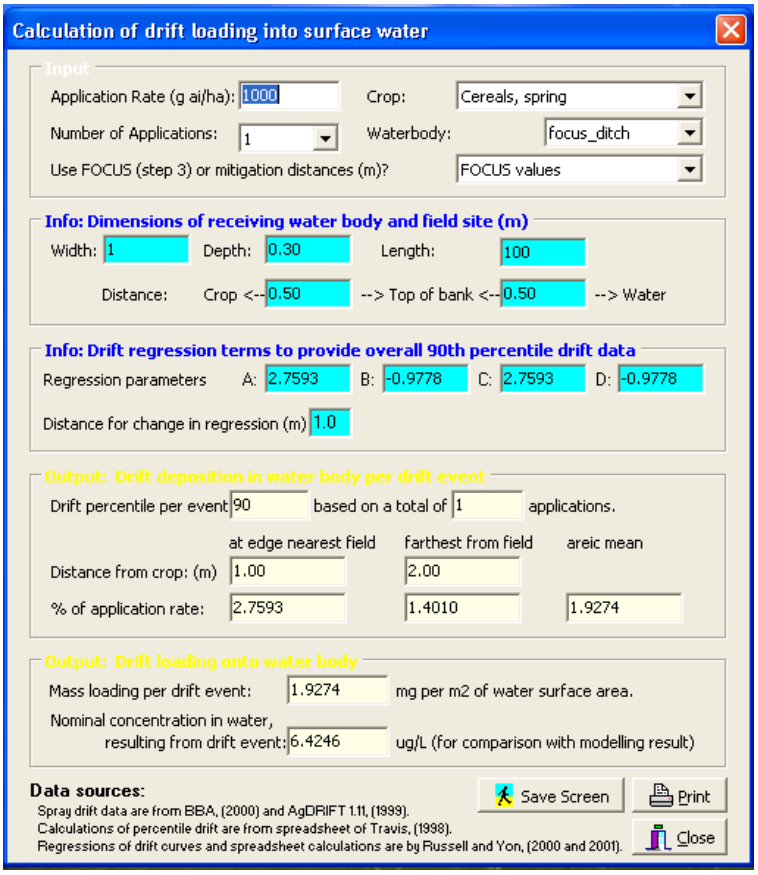

Figure 2.31. The FOCUS Drift Calculator.

For FOCUS streams, the mean deposition and mass loading, as calculated by the FOCUS Drift Calculator, have been multiplied by a factor 1.2 to account for pesticide mass incoming from the upstream catchment as decided by the FOCUS Surface Water Scenarios Working Group.

If mitigation measures are to be considered, for example in FOCUS Step 4, then the user can specify the width of the buffer zone. In the field for 'Use FOCUS (Step 3) or mitigation distances', the user can select the width of the buffer zone to be considered. In the 'output' sections of the 'Calculation of drift' form, the value for the deposition of pesticide onto the water body expressed as a percentage of the application rate as well as that for the areic deposition on the water body are given taking into account the width of the buffer zone as specified by the user.

The effect of spray drift mitigation by buffer zones on exposure concentrations in surface water can be evaluated using FOCUS_TOXSWA. The value for the areic deposition as calculated by the Drift Calculator in SWASH has to be taken to set the pesticide loadings parameter in the TOXSWA input file.

3 Installation and getting started

3.1 Installation

The SWASH software package can be downloaded from the FOCUS web site: http://focus.jrc.ec.europa.eu/sw/index.html. The installation procedure results in the installation of SWASH_5.3. The installation directory is C:\SWASH by default. The MACRO, PRZM and TOXSWA software packages compatible with SWASH_5.3 should be installed in the same directory, i.e. C:\SWASH\MACRO, C:\SWASH\PRZM and C:\SWASH\TOXSWA respectively. The installation directory of SPIN and of its database is free (but do not install at a network drive). SWASH works only correctly if it is installed in the root of a hard drive. The drive letter may also be another drive letter than C.

FOCUS_SWASH_5.3 has been tested on Windows Vista, Windows 7 and 8. SWASH is likely to run on previous versions, however, this has not been tested. For the installation it is necessary to have Administrator rights.

SWASH requires 12.5 Mb for installation. A monitor with at least a screen resolution of 1024x768 is required, using 256 colours. Use 'small fonts' as display setting. The faster the processor the better.

The Read_me_first file that is supplied with the installation package contains the information for installation of FOCUS_SWASH_5.3.

It should be noted that if FOCUS_SWASH_3.1 has already been installed then it is not possible to reuse the SWASH database because the database is no longer an MS Access database, and the data of the substances are now stored in a separate database (SPIN).

Note that if an user utilizes a SWASH database containing a project with a substance that is not listed in SPIN, then an error will be shown in SWASH. After such a project is deleted, SWASH will work properly.

3.2 Getting started

The first step to perform a FOCUS Surface Water run consists of editing the properties of a substance that is already present in the SPIN database or the creation of a new substance.

Once the substance is included in the SPIN database, the FOCUS wizard or the User-defined wizard can be used to create the runs required in the assessment of the fate of the substance in the surface water.

If in the FOCUS wizard form or the User-defined wizard form the substance is followed by a parenthesis containing the words 'incomplete' or 'ambiguous', the user is informed that either not all values for the required parameters have been entered in SPIN or that the substance has a soil metabolite scheme not supported within the current FOCUS surface water models. Both the FOCUS wizard and the User-defined wizard can be used to check whether a substance has been properly created in SPIN for running the FOCUS surface water models.

Using the FOCUS wizard the user can only select the substance and one crop of interest. Using the User-defined wizard, the user can select only one substance, but also one or more crops, one or more (up to 3) water body types and one or more (up to 10) scenarios.

After creation of the project with either the FOCUS wizard or the User-defined wizard, the user has to enter the correct application data on the 'Applications' form. Once the application data have been entered for the runs created in the new project, the user has to export the data to the MACRO and PRZM shells. No export is needed for TOXSWA because it uses the same database as SWASH.

This sequence of steps is depicted in Figure 3.1.

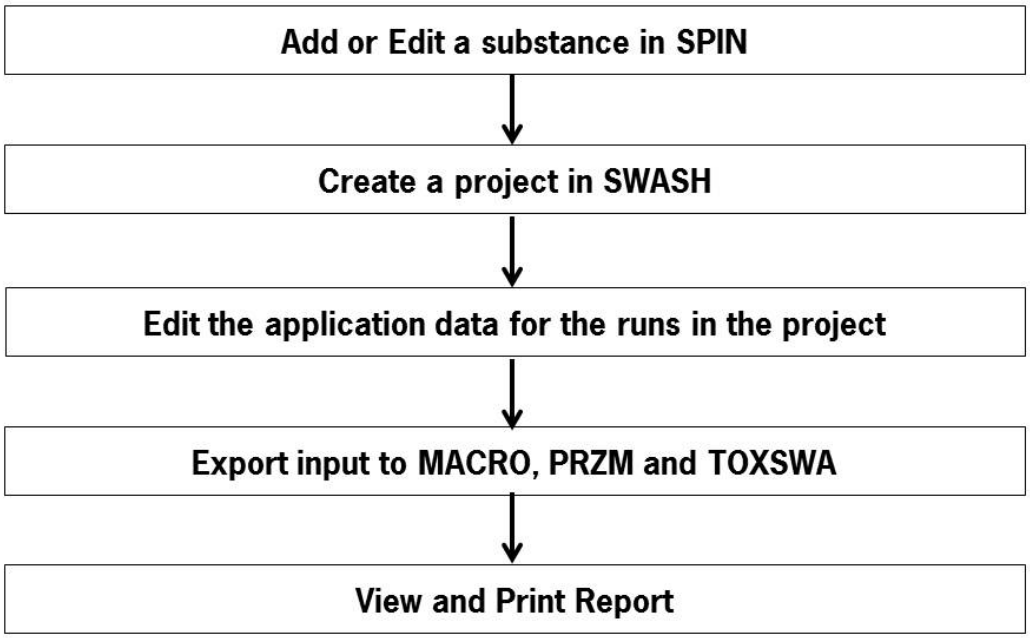

Figure 3.1 Scheme for preparing input to run FOCUS Surface Water Scenarios using SWASH.

For a drainage scenario first a run with MACRO has to be executed before running TOXSWA. After starting the MACRO shell using the 'MACRO' button on the main window of SWASH, the user has to specify in the MACRO shell the run that has already been created in SWASH. The report of the SWASH project can assist the user in specifying the correct scenario, crop, parent compound and application data. In particular it is important to select the application data for the relevant run. Each application scheme has a unique ID (the runID). The application scheme with the same runID as that for the corresponding run as defined in SWASH should be taken. After running MACRO the user has to process the output using the FOCUS_MACRO shell to create the m2t file containing the input of the drainage and pesticide fluxes that will be used by TOXSWA.

The sequence of steps to specify and to execute a drainage scenario run with MACRO are also shown in Figure 3.2.

For a run-off scenario first a run with PRZM has to be executed before running TOXSWA. After starting the PRZM shell using the 'PRZM' button on the main window of SWASH, the user has to import the SWASH project with the runs of interest. Next, a crop has to be selected from the list of crops in the SWASH project. After confirmation of this selection the input files for PRZM can be created by clicking on 'Write' of the 'PRZM in FOCUS' window. The PRZM shell returns the message 'output files successfully written' and thereafter the PRZM runs within this project can be executed. PRZM automatically prepares the p2t file containing the run-off and erosion fluxes input for TOXSWA. The steps to be followed when defining a run for a run-off scenario are summarized in Figure 3.3.

The last part of execution of a run for a FOCUS Surface Water Scenario is to perform simulations with TOXSWA. The TOXSWA shell can be started after clicking of the 'TOXSWA' button. The steps to be followed are shown in Figure 3.4. It should be noted that for Step 3 calculations the drift deposition loadings are calculated automatically by SWASH and written to the TOXSWA input file. The drain water fluxes and pesticide loadings are read from the m2t file and the run-off water and erosion fluxes and the pesticide loadings via run-off or erosion are read from the p2t file.

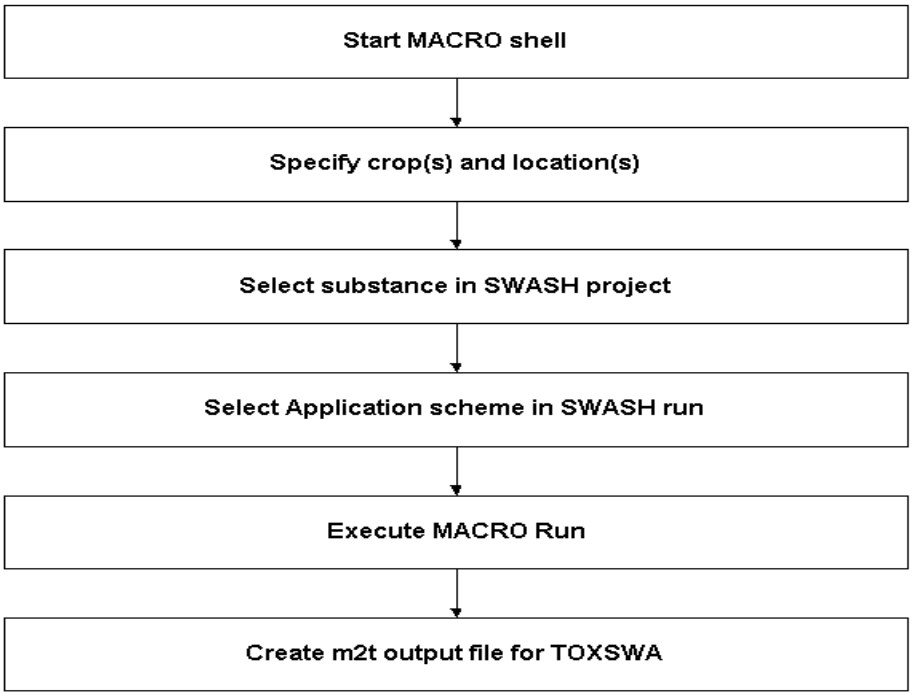

Figure 3.2. Scheme for executing a run with MACRO for a drainage scenario.

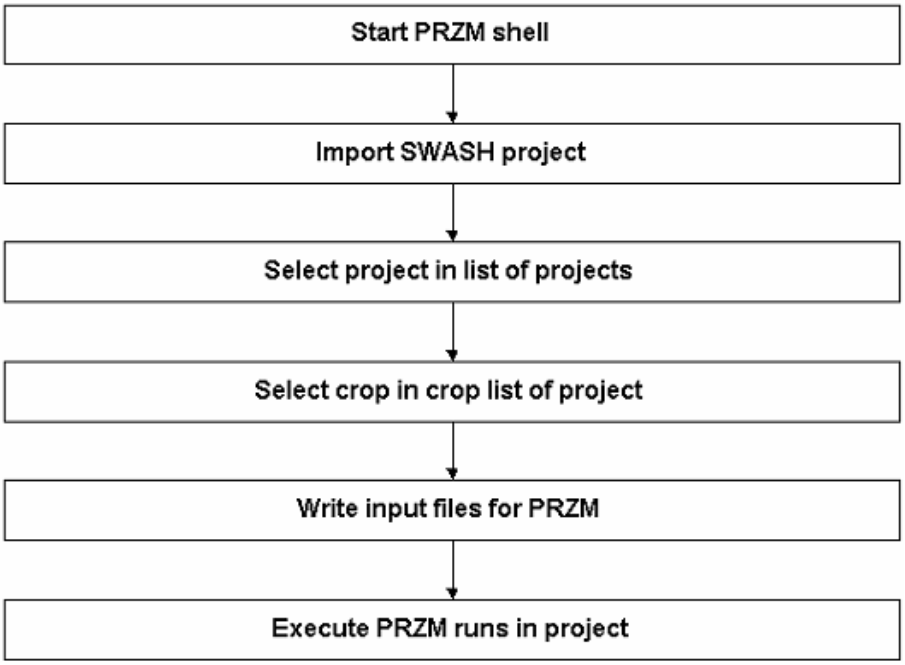

Figure 3.3. Scheme for executing a run with PRZM for a run-off scenario.

Once the TOXSWA runs in the project have been completed, the target data on the exposure concentrations around found in the summary output file of TOXSWA (Beltman *et al*., 2014).

It should be noted that the highest areic deposition resulting from spray drift at any time occurs for a single application. For multiple applications, the areic deposition rate per event is smaller (Ganzelmeier *et al*., 1995). Therefore, it is recommended to always perform an exposure assessment with TOXSWA for a single application with the highest application rate.

More detailed information on the TOXSWA model and guidance on how to use FOCUS_TOXSWA is given in the User's manual of FOCUS_TOXSWA (Beltman *et al.,* 2014).

Support for SWASH can be requested by sending an email to swash@pesticidemodels.eu.

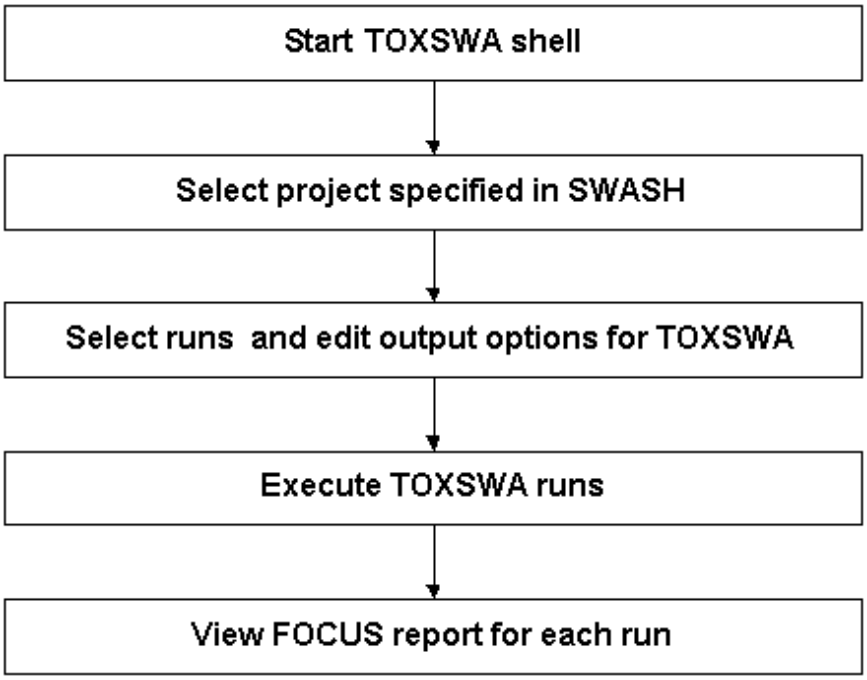

Figure 3.4. Scheme for executing a run with TOXSWA scenario.

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Justification

This manual is an update of the manual of FOCUS_SWASH 4.2 (Fait *et al.,* 2013). The manual is updated because the SWASH database and user interface have been adapted resulting in FOCUS_SWASH version 5.3. The content of this report was reviewed by Mechteld ter Horst of Alterra Wageningen UR. The project was supervised by Jennie van der Kolk (contact of WOT N&M, theme Agri-Environment) and seen and approved by Anja van Gemerden (Ministry of Economic Affairs)

Annex 1 Creating a new substance in SPIN

To create a new substance the following steps are needed:

1. Start SWASH

2. Click the button 'View and Edit Substances'. The SPIN database window is shown.

3. Click the button  to add a substance. The 'New Substance' window is shown. It is also possible to copy an existing substance () and modify the parameters (in fact for FOCUS surface water scenario calculations it is advised to always copy EXSW0).

4. Enter a unique code and name for the new substance you are about to define and click on  to save the changes.

5. Enter all the required parameters for running the FOCUS surface water models. Parameters not required for FOCUS surface water calculations are shown in grey.

Annex 2 Example of a SWASH report

```
* SWASH report file
* made by FOCUS-SWASH UI v. 5 (internal version 5.1.0, 02 April 2015)
*
* File Name   : c:\SwashProjects\Project_1\Project_1_report.txt
* Description : Example project 1
* Substance   : EXSW2
*
* Creation    : 29-May-2015, 08:54
*
* Remarks : SWASH report helps you to set up the needed runs to calculate the PECsw and PECsed, occuring in the EU
*           for the selected substance, used on the selected crop. The scenario code informs you which models you need to
*           run for this scenario.
*           D1-D6: drainage entries calculated by the MACRO model, fate in surface water calculated by the TOXSWA model
*
*           R1-R4: runoff and erosion entries calculated by the PRZM model, fate in surface water calculated by the TOXSWA model
*
*
*           For STREAMS the Mean Deposition and Mass Loading, as calculated by the FOCUS Drift Calculator, have been multiplied by a
*           factor 1.2 to account for pesticide mass incoming from the upstream catchment as decided by the FOCUS Surface Water
*           Scenarios Working Group.
*
*
*****************************************************************************************************************************
*  CREATED RUNS
*****************************************************************************************************************************
*
*                                                  |--------------- APPLICATION -----------------|----- on Water Surface -----|
* -ID------Crop(1st/2nd)-------Scenario-WaterbodyType-|-Method--------First/Last/Interval--#---Rate-|-Mean Deposition-Mass Loading
*                                                                          (d)          (kg/ha) (% of Appl. Rate)    (mg/m2)
*
* 1     Cereals, winter(1st)     D4_Pond               ground spray   8-Sep /28-Oct/7      1  1.0000       0.154           0.154
*                                                                                          2  0.7500       0.154           0.116
*                                                                                          3  0.5000       0.154           0.077
*
* 2     Cereals, winter(1st)     D6_Ditch              ground spray   16-Nov/16-Dec/1      1  1.0000       1.927           1.927
*
* 3     Cereals, winter(1st)     R1_Stream             ground spray   29-Oct/28-Nov/1      1  1.0000       1.716           1.716
*
********************************************** Surface WAter Scenarios Help **********************************************
```

Annex 3 Day of the year calender

Day in Month	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
January	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
February	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59			
March	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90
April	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	
May	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151
June	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	
July	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212
August	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243
September	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	
October	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304
November	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	
December	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365

Annex 4 Addendum to update the manual of FOCUS_TOXSWA 4.4.2 for FOCUS_TOXSWA 4.4.3

This form intends to update the manual of FOCUS_TOXSWA 4.4.2 (Beltman *et al*., 2014) for FOCUS_TOXSWA 4.4.3. While FOCUS_TOXSWA 4.4.2 could only account for the formation of one metabolite in the water of the upstream catchment of FOCUS stream scenarios, this new FOCUS version of the TOXSWA model can handle the formation of more metabolites in one simulation. FOCUS_TOXSWA 4.4.2 was submitted to the FOCUS Version Control Group (http://focus.jrc.ec.europa.eu/), but never released. By substituting the changes described in this form into the manual of FOCUS_TOXSW 4.4.2 the manual is valid for version 4.4.3.

The correction factors for metabolite formation in the upstream catchment of the FOCUS stream scenarios are substance-specific as well as scenario-specific. They are calculated by FOCUS_SWASH with the aid of the degradation rates of the parent and of the metabolite and a conservative estimate of the residence time in the upstream catchment of the scenario. They are stored in the database of FOCUS_SWASH, from where they are retrieved in the TOXSWA-GUI

Updated parts of Section 3.3.10 of the FOCUS_TOXSWA 4.4.2 manual: Section 7 Management

The updates below refer to (i) the text under the subheading Metabolite formation in water in upstream catchment and (ii) part of Figure 3.7.

Metabolite formation in water in upstream catchment
In the upstream catchment of FOCUS stream scenarios metabolites are formed in molar fractions varying between 0 (no metabolite formation) and 1 (1 mol parent has been transformed into 1 mol metabolite). A factor, CFm,up (FraMetForUps), is needed to account for this. This correction factor is specific for the metabolite, the substance and the scenario (because of the temperature as well as the time spent in the upstream catchment during which the metabolite can be formed). The correction factor accounts both for metabolite mass formed from parent mass deposited by spray drift on the water surface area in the upstream catchment, and for metabolite mass formed from parent mass originated from drainage or runoff in the upstream catchment. See Adriaanse *et al*. (2014) for the theoretical basis of this correction factor and the procedure to calculate it. Because these correction factors depend on the substance as well as the scenario they have been incorporated in the management section of the input file (see Figure 3.7).

```
*-------------------------------------------------------------------------------
*
* Section 7: Management section
*-------------------------------------------------------------------------------
*
.


.
* If: CallingProgram = FOCUS and OptWaterSystemType = WaterCourse
Yes         OptUpsInp              ! Switch for upstream catchment treated (Yes, No)
0.          RatAreaUpsApp (-)      ! Ratio of upstream catchment treated [0.0 - 1]
0.774       FraMetForUps_MWP1 (-)  ! Correction Factor primary metabolite upstream catchment
0.957       FraMetForUps_MWP2 (-)  ! Correction Factor primary metabolite upstream catchment
```

Figure 3.7. Excerpt of the Management section in the TOXSWA input file showing the correction factor for metabolite formation in the upstream catchment of FOCUS stream scenarios, $CF_{m,up}$ (`FraMetForUps`)*. In this example two primary metabolites are formed, MWP1 and MWP2.*

Updated parts of Section 4.4.4 of the FOCUS_TOXSWA 4.4.2 manual: Special cases: metabolite formation in the upstream catchment of FOCUS streams

The updates below refer to Figure 4.3 and its three-lines description given above this figure. In addition the last two sentences of this section can be deleted: "The entry of this factor for FOCUS Step 3 runs..... , i.e. a conservative estimate."

In the TOXSWA_GUI the correction factors CFm,up can be viewed (FOCUS Step 3 calculations) or entered or changed (FOCUS Step 4 calculations) at the Edit runs form accessed via the Entries tab, in the section Upstream catchment entries (Fig. 4.3a). By clicking the button CF the CF form can be accessed (Fig. 4.3b).

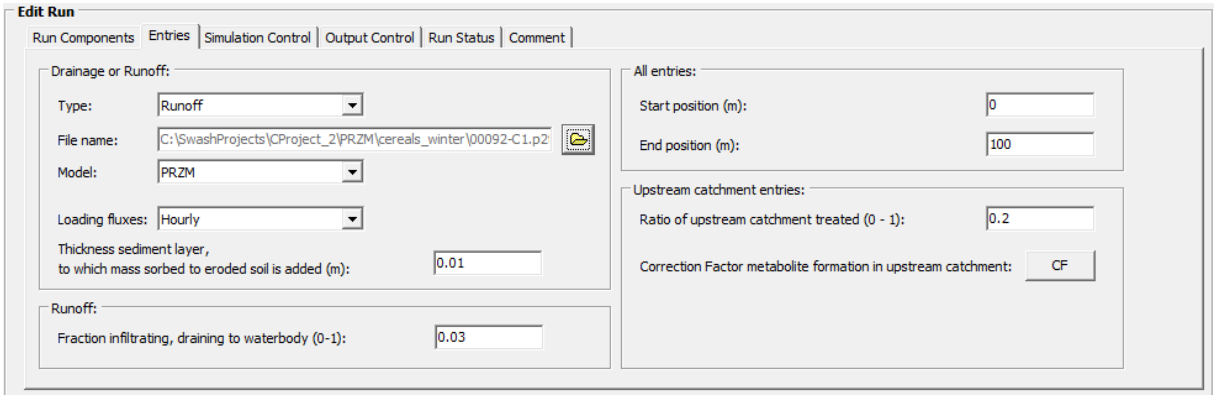

Figure 4.3a Entries tab of the Edit runs form. The section Upstream catchment entries contains the button CF; after clicking on it the correction factors for formation of primary water metabolites in the upstream catchment of FOCUS stream scenarios are shown.

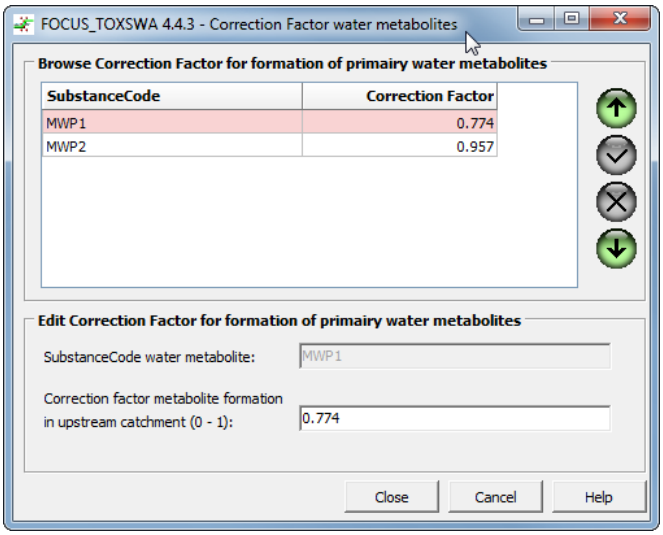

Figure 4.3b Browse Correction Factor water metabolites form.

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