SWASH Manual 2.1

User's Guide version 2

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Preface

End 1997 the FOCUS Surface Water Scenarios Working Group started her activities. The Group developed a tiered approach to estimate pesticide exposure concentrations, which has been submitted to the Working Group on Pesticide Legislation of the European Union. Since 2003, the calculated concentrations in the FOCUS Surface Water Scenarios have become part of the EU review process for plant protection products according to EU Directive 91/414/EEC. 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 and from September 1999 to April 2003 SWASH, acronym for Surface WAter Scenarios Help, was developed by Erik van den Berg and Paulien Adriaanse from Alterra (CWK-ERA), in co-operation with Johnny te Roller and Daniel van Kraalingen from Alterra (CGI-Systems). Nick Jarvis (Swedish Univ. Agric. Sci., S) for MACRO and Mark Russell (Dupont Crop Protection, USA) and Mark Cheplick (Waterborne–env., 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 has been financed by various sources. In 2000 the ECPA (European Crop Protection Agency) procured 20 000 €, and the Dutch Ministry for Agriculture, Fisheries and Nature Management also allocated 19 000 € for SWASH. In 2001 DG SanCO from the EU contributed 38 000 € to SWASH. All other work on FOCUS_SWASH_1.1 in 2002 and 2003 and the work on the release of FOCUS_SWASH_2.1 has been financed by the Dutch Ministry of Agriculture, Nature and Food Quality within Research Programme 416 "Pesticides and the environment".

The current document (WOt-werkdocument 83) is the user's manual of FOCUS_SWASH_2.1. This version is an updated version of the manual of FOCUS_SWASH_1.1 (2005).

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 (Alterra rapport 508), explaining the technical design of the SWASH database, the SWASH user interface and the communication and installation procedures. This document is needed for possible, future extensions or updates.

SWASH project team

Contents

Summary

A tiered approach has been developed to assess pesticide exposure in the EU FOCUS scenarios for surface waters. In Step 3, a drift assessment tool, models to calculate pesticide input into the surface water and a model to assess the fate in the 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_1.1.1, calculating pesticide entry into surface water through run-off
- FOCUS_MACRO_4.4.2, calculating pesticide entry into surface water through drainage
- FOCUS_TOXSWA_2.2.1, calculating the fate of pesticides in surface waters.

To facilitate the calculation of exposure concentrations at 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:
- Maintenance of a central pesticide properties database,
- 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, it helps the user to determine which runs need to be performed for pesticide applications to various crops, and it defines projects and runs for MACRO, PRZM and TOXSWA that can be selected for execution after starting the corresponding shells.

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 91/414/EEC (FOCUS, 2001). To carry out these exposure assessment scenarios for surface waters, a drift assessment tool and two pesticide fate models have to be run in the correct sequence (see 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_1.1.1, calculating pesticide entry into surface water through run-off
- FOCUS_MACRO_4.4.2, calculating pesticide entry into surface water through drainage
- FOCUS_TOXSWA_2.2.1, calculating the fate of pesticides 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 4.4.2 includes the MACRO model version 4.3b. This version contains some improved process descriptions (e.g. snow pack, Freundlich sorption) and 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. The PRZM in FOCUS version is based on PRZM version 3.21β. PRZM can describe three transformation schemes and up to two metabolites: 1) a parent with one metabolite, 2) a parent with 2 sequential metabolites and 3) a parent with 2 metabolites.

The TOXSWA model describes the behaviour of pesticides in small water bodies. Processes considered are sorption, transport, volatilisation and transformation. TOXSWA version 1.2 (Adriaanse, 1997; Beltman and Adriaanse, 1999) is used to simulate water bodies with constant discharge and water depth. 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. This version contains a Help utility and all reported bugs for FOCUS_TOXSWA_1.1.1 have been repaired.

To assist the users of the FOCUS Surface Water Scenarios at 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 (Fig. 1.1). The aims for the development of SWASH were to maintain a central pesticide properties database, 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.

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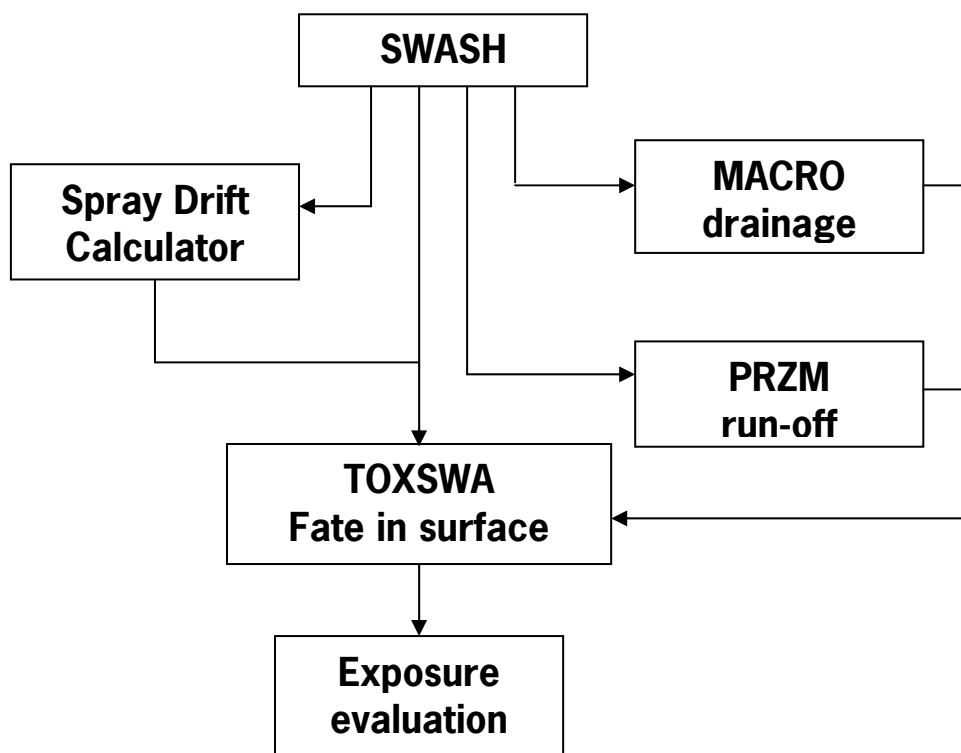
Figure 1.1: Sequence of tools and models used to calculate pesticide exposure in the proposed Step 3 EU FOCUS Surface Water Scenarios.

2 User's guide for the SWASH User Interface

The handling of the FOCUS Surface Water Scenarios has become 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 development of a tool to execute FOCUS runs in an easy and user-friendly manner, has resulted in the SWASH software package. 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 use of the substance database is done 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

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 and this is shown in Figure 2.1.
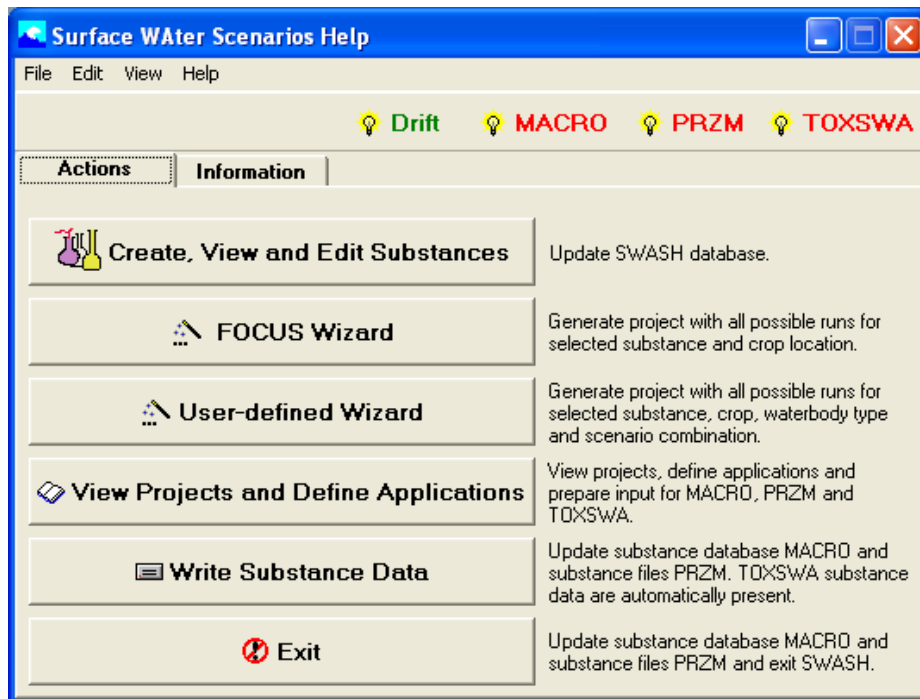
Figure 2.1: The main screen of the SWASH interface with the 'Actions' tab displayed.

The 'Actions' page contains six 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 substance form, where the user can enter new substances or modify the properties of substances already present in the database. The test substances as defined by the FOCUS Surface Water Group are available in the database upon installation. However, the properties of these substances are fixed and they 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 are 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 user overviews 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 the runs selected by the user. The user can also print a text report of the specifications of the runs in a project (See section 2.1.4).

The button 'Write substance data' will update the MACRO substance database and the PRZM file with substance data for any changes in the substance database of SWASH. For TOXSWA this is done automatically, because TOXSWA uses the same database as SWASH.

Using the 'Exit' button, the user can end a SWASH session. When exiting the MACRO substance database as well as the PRZM file with substance data will be updated.

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 assessment, but no changes are made in the database, or input prepared for the other models. This will be described in more detail in section 2.2.

2.1.1 The Substance Screen

The substance screen gives access to the pesticide database of SWASH. On the substance screen the user can enter new substances or modify the properties of substances already present in the database. Substances entered here, will be transferred to the MACRO substance database and the data file containing the substance data for PRZM. Substances that were entered into the MACRO database independently from SWASH, will be included in the SWASH substance database when exiting the MACRO shell or starting SWASH. TOXSWA makes direct use from the SWASH database. Guidance for defining the substance properties is given in FOCUS, 2001 (sections 7.3 and 7.4), but also below.

In Figure 2.2 the substance screen is shown. The upper part consists of a 'browse' part in which the user can browse the list of substances using the scroll bar on the right. In the lower part there are four tabs. In Figure 2.2 the 'General' tab is shown.

Figure 2.2: The substance form of SWASH – The general section

On the 'General' tab the user has to specify the general physico–chemical properties of the substance. The units in which the data must be introduced in the form are shown next to the field where a value has to be entered. It should be noted that the units for these properties are the units as used in SWASH. The units of the same properties in the PRZM and MACRO shells are in many cases different. However, when transferring substance data between SWASH and MACRO and between SWASH and PRZM the values as entered in SWASH will be converted to the correct values for MACRO and PRZM.

The code refers to the unique code that the user has to attribute to the substance, which is used in the SWASH database to identify this substance. The name field refers to the name (not necessarily unique) the user has to give to the substance.

The saturated vapour pressure must be specified in Pa and the temperature at which this value was obtained should be given in degrees Celsius. The range in the saturated vapour pressure for pesticides is very wide. Therefore, for each substance the value should be looked up in a Handbook on chemical properties of pesticides (See e.g. Tomlin, 2003, Hornsby *et al.*, 1996). The saturated vapour pressure depends on the temperature, its dependency is described on the basis of the Van 't Hoff equation for equilibrium reactions. Therefore, a value for the enthalpy of vaporisation must be given in J mol^{-1}. In a literature study, Smit *et al.* (1997) reported the enthalpy of vaporisation to range from 58000 to 146000 J mol^{-1} using data for 16 pesticides. The FOCUS Surface Water group has adopted a default value of 95000 J mol^{-1}.

The water solubility must be given in mg L^{-1} and the temperature at which this value was obtained must be given in degrees Celsius. Values for the water solubility are reported in Tomlin (2003) and Hornsby *et al.* (1996). As the water solubility is affected substantially by the temperature, its dependency on this factor is described on the basis of the Van 't Hoff equation for equilibrium reactions. Therefore, a value for the enthalpy of dissolution must be given. The FOCUS Surface Water group has adopted a default value of 27000 J mol^{-1}.

The coefficients of diffusion of the substance in water and air must be given in m^2 d^{-1}. The default values adopted by the FOCUS Surface Water group are 0.43 10^{-4} and 0 43 m^2 d^{-1}, respectively (FOCUS, 2001). A more accurate value for these coefficients can be made using an estimation method described by Reid and Sherwood (1966).

A useful functionality on the 'Substance' screen is that it is easy to make a copy of a substance. After clicking on 'Copy', a copy will be made of the substance selected, except that the substance code and the substance name will be different. Then, the user has to adjust the code and the name of the substance. Next the user has only to modify those values that are different from the values for the original substance.

Other buttons on this form are the 'New' button in order to add a new substance to the database, and a 'Remove' button to remove a substance from the database. Creating a new substance is explained in Annex 1. To create a metabolite, unselect the option 'Parent' as shown in Figure 2.2. In order to add a metabolite to a parent, press the button 'set Metabolites'.

The 'Save' button is to save the modifications in the properties of the substance in the SWASH database, and the 'Undo' button is to undo the modifications entered.

The test substances as defined by the FOCUS Surface Water Group are available in the database upon installation. It should be noted that the properties of these substances are fixed and they cannot be modified.

To specify a new or to edit an existing transformation scheme the user should go to the 'Metabolite scheme' form by clicking on the button 'set Metabolites' in the top right corner of the 'General section' tab. The possible options for transformation schemes for MACRO differ from those for PRZM. The form is shown in Fig. 2.3

Figure 2.3 The metabolite scheme form of SWASH – transformation schemes in MACRO and PRZM

In PRZM the user can choose between three different transformation schemes. After selecting the required scheme, the fields for the data needed will be shown in the lower part of the form. In the example shown below, the user has identified substance 6m_sw as the only metabolite for substance 6_sw. Next the user has to specify the molar fraction of parent 6_sw that will be transformed into metabolite 6m_sw.

In MACRO the user can choose between two different transformation schemes. After selecting the required scheme, the fields for the data needed will be shown in the lower part of the form. Next the user has to specify the mass fraction of the parent 6_sw that will be transformed into the metabolite.

The sorption section of the 'Substance' form is shown in Figure 2.4. In this section the user can select between the sorption options 'General' and 'Detailed'. If the 'General' option is selected, then the user has only to enter either the K_{oc} value or the K_{om} value. The value of the K_{om} will be automatically calculated from the K_{oc} and vice versa. FOCUS recommends a conversion factor of 1.724: $K_{oc} = 1.724 \cdot K_{om}$. (FOCUS, 2000). This conversion factor is used in SWASH. The K_{oc} or K_{om} value will be used as the value for the sorption coefficient in all solids, i.e. soil, suspended solids and sediment.
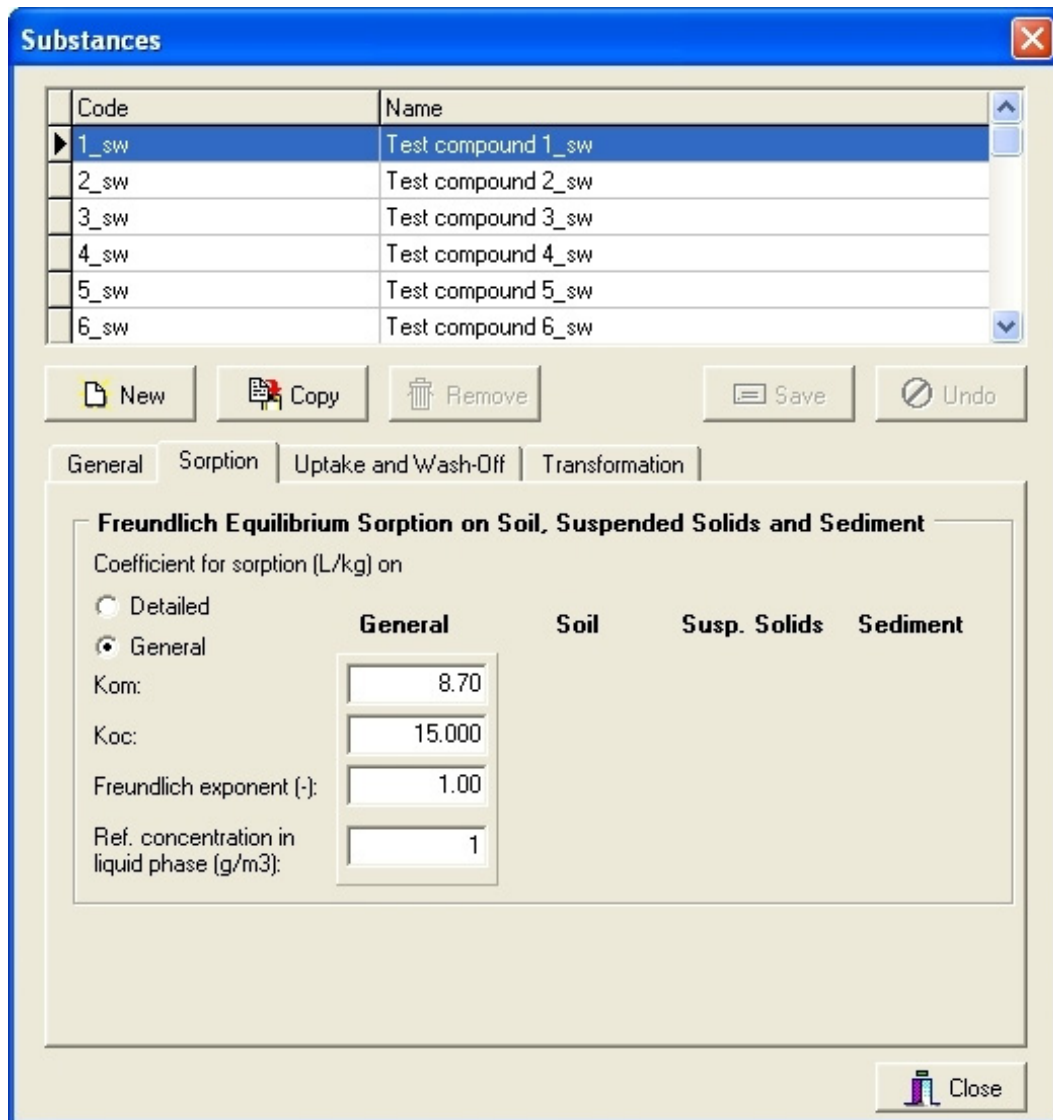
Figure 2.4: The substance form of SWASH – The sorption section

If the 'Detailed' sorption option is selected, then the user has to enter separate K_{oc} or K_{om} values for soil, suspended solids and sediment. The user can choose the sorption isotherm using the value for the Freundlich exponent. If this exponent is set to 1, then a linear sorption isotherm is used. If the exponent is not equal to 1, the sorption is described with the Freundlich equation. The reference concentration is introduced into the Freundlich equation to obtain a Freundlich coefficient independent of the value of the exponent. The value of the reference concentration should be within the range of concentrations in the measurements on which the Freundlich sorption coefficient is based. In most studies, the value of this concentration is set to be $1.0 \cdot 10^{-3}$ kg m^{-3} (1.0 mg dm^{-3})

The uptake and wash-off section of the 'Substance' form is shown in Figure 2.5. In this section the user has to specify the factor for the uptake of the substance by the plant roots in the soil and the factor for the wash-off of the substance from the plant leaves.

The coefficient for the uptake by plant roots is also described as the transpiration stream concentration factor, F. For non-ionic pesticides, this factor can be estimated from the octanol-water partitioning coefficient as described by Briggs *et al*. (1982). For these pesticides this factor will always be between 0.0 and 1.0. For ionic pesticides no reliable estimation methods are available and the factor may be greater than 1.0. Shone and Wood (1974) reported a value of 3 for the anion of 2,4-D.

Figure 2.5 The substance form of SWASH – The uptake and wash-off section

The user has to enter different values for the foliar wash-off factor to be used in PRZM or MACRO. The default value is 0.5/cm in PRZM and this is equivalent to the default value of 0.05/mm for MACRO. The default value is appropriate for moderately to highly soluble pesticides. If the solubility is lower than about 8000 mg L^{-1} then the value for the wash-off coefficient should be recalculated using the empirical equation of Wauchope *et al*. (1997) as explained in FOCUS (2001). Please note that the wash-off factor for a metabolite is not relevant, because it is disabled in SWASH.

The transformation section of the 'Substance' form is shown in Figure 2.6. In this section the user has to specify the half-lives of the substance in all the compartments considered, i.e. the water layer of the water body, the soil system, the sediment system in the water body and the crop on the field next to the water body. For the first three compartments the temperature at which the half-life has been obtained must be specified.

The half-life of transformation depends strongly on the pesticide and the environmental and soil conditions. Values for the half-life of 243 pesticides have been reported by Linders *et al.* (1994).

Water-sediment studies can be used to obtain data on the transformation half-life in water and sediment. Key elements for such studies as well as guidance on the procedure to derive the DT50 for the water layer and the sediment are given by FOCUS (2001).

Figure 2.6: The substance form of SWASH – The transformation section

For the half-life on the crop the temperature is not needed, because there is not enough knowledge how to describe the temperature dependency of the half-life of the substance on the crop. A recent EU guidance document on bird and mammal risk assessment (SANCO/4145/2000, 2002) recommends that a default value of 10 days be used as a reasonable default value for foliar half-life. To maintain harmonisation between guidelines, a default foliar half-life value of 10 days is also recommended for use in FOCUS surface water modelling. If appropriate experimental data is available to support a significantly different foliar dissipation rate, this value can be substituted for the default value. Please note that the half-life for a metabolite on the crop is not relevant, because it is disabled in SWASH.

After clicking on the 'Specifications on transformation in soil ...' button, a form appears on which additional data has to be entered related to the transformation in soil. The contents of this form is presented in Figure 2.7. The input data required by PRZM for the effect of the soil water content on the transformation are different from the data required by MACRO. The effect of the moisture content on the rate coefficient of transformation can be described with an equation based on Walker (1974). For the FOCUS surface water scenarios this parameter is set to 0.7. For MACRO, the moisture content of the soil in the transformation experiment has to be entered as a pF value. For PRZM, the moisture content is expressed either as an absolute value on mass basis or as a percentage of the moisture content at field capacity. Further, the check box for 'Use bi-phase degradation' is not marked by default, so there is no bi-phasic degradation in PRZM runs with this substance. As a substance might be used in all scenarios, values must be entered in all fields if no default is given by SWASH. Please note that for a metabolite the bi-phase degradation is not available and therefore is disabled.

Figure 2.7: The substance form of SWASH – Specification on the transformation in soil.

2.1.2 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 screen, the form shown in Figure 2.8 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.
- The substance to be assessed; the substance can be selected from the list of substances present in the database. The list is shown by clicking on the button with the arrow on the right-hand side of the 'Substance' field.
- 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.
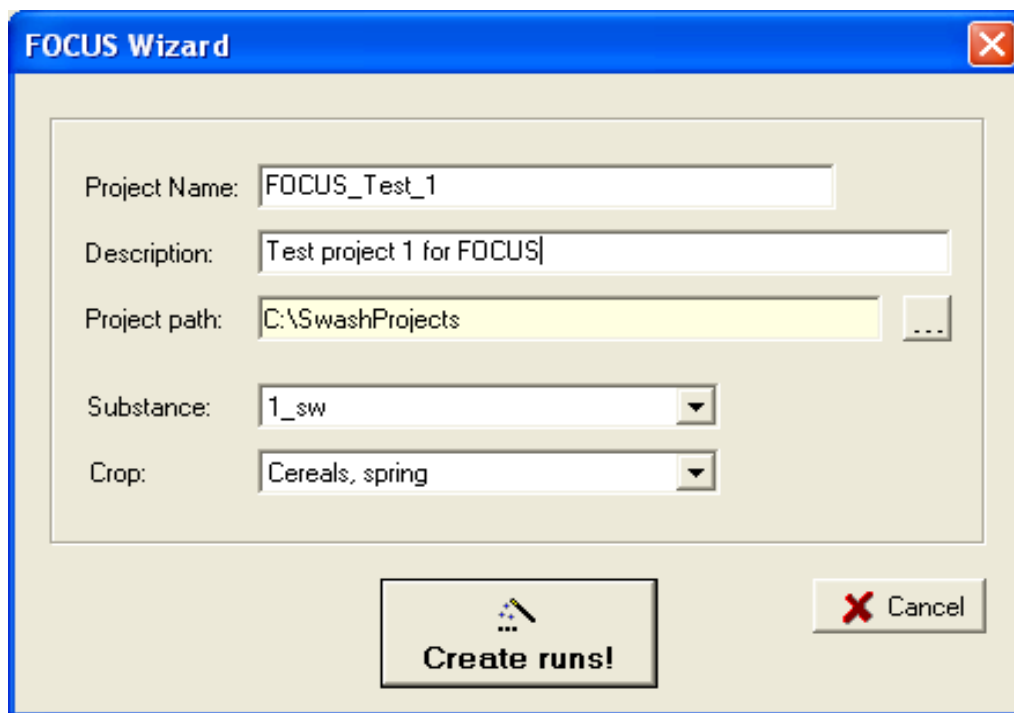
Figure 2.8: The FOCUS wizard

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, the user gets information in a separate window how many runs have been created. After clicking on 'OK' the main screen 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 here after exporting data to PRZM and MACRO (See section 2.1.4).
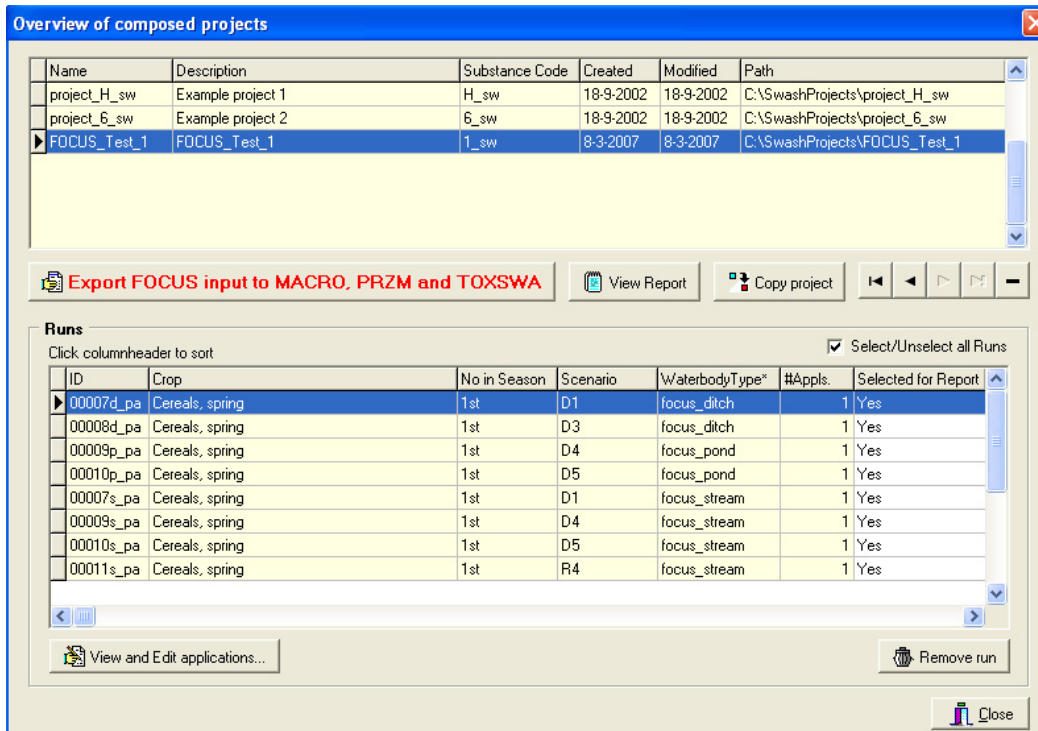
Figure 2.9 : Overview of the projects and the runs in the project selected.

The user can get an overview of the runs created by clicking on the button 'View projects and define applications'. An example of the 'Overview of composed projects' form of SWASH is shown in Figure 2.9. In the upper part of the form the projects created in SWASH are listed. For the project selected (indicated by '►' on the left-hand side of the 'Name' column), i.e. the project 'FOCUS_Test_1, the runs created are listed in the lower part of the form. After clicking on the 'View and Edit applications' button, the form shown in Figure 2.10 is shown on the screen.
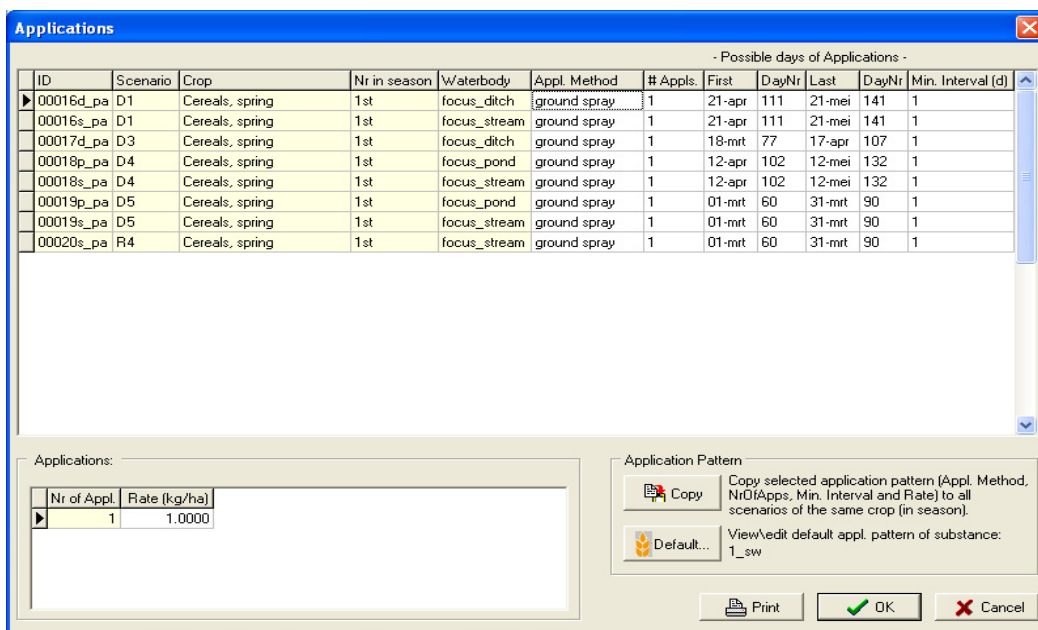
Figure 2.10: Detailed description of the runs in a project.

The forms shown in Figures 2.9 and 2.10 are explained in detail in section 2.1.4.

It should be noted that the user will have 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).

2.1.3 The User-Defined wizard

After clicking on the button 'User-defined Wizard' on the main screen, the first form of the Wizard is displayed on the screen. On this form, shown in Figure 2.11, the user has to select the substance for which he 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.
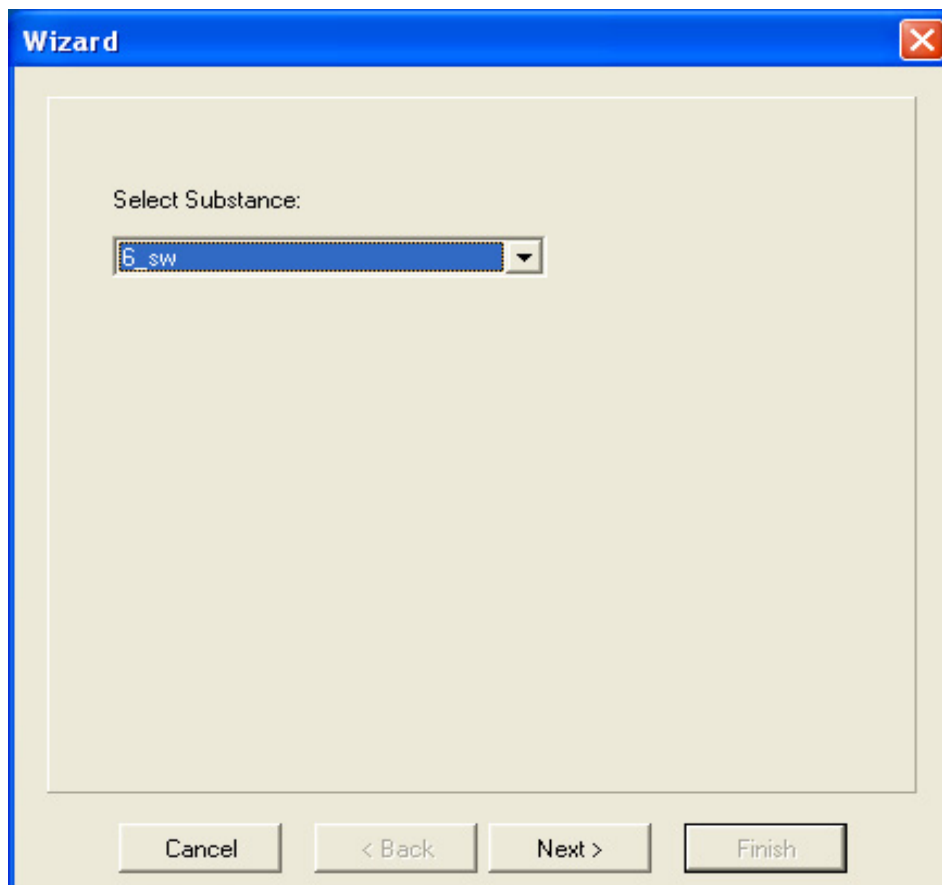

Figure 2.11: The User-Defined Wizard – Substance

After selection of the substance, the user has to click on the 'Next' button. Then the form presented in Figure 2.12 is shown on the screen. In the example, the user has selected 5 crops: spring oil seed rape, maize, legumes, hops 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 2.12: 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 and this form is shown in Figure 2.13.
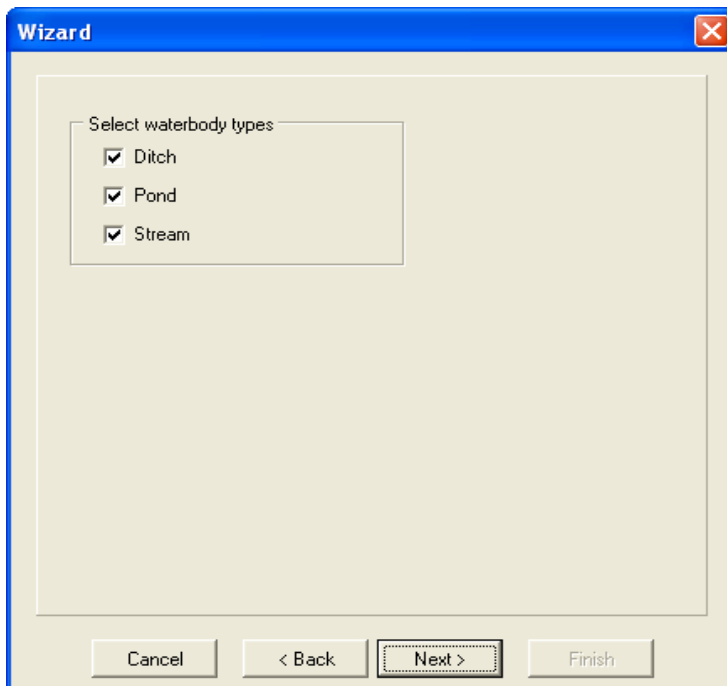
Figure 2.13: The User-Defined Wizard – Water bodies

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 name.

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 2.14, the scenarios D3, D4, D5 and R2 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.
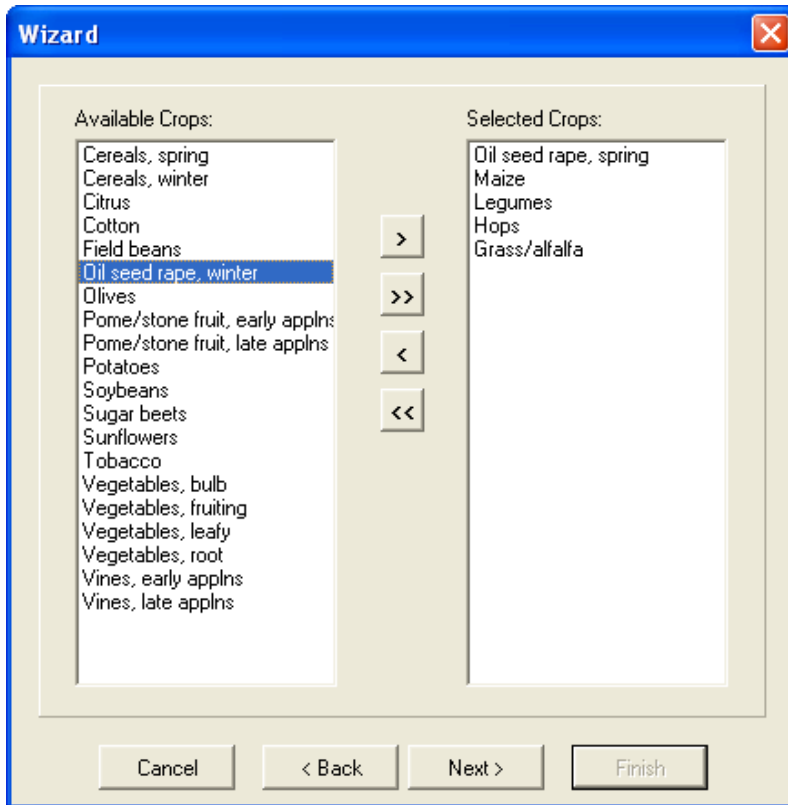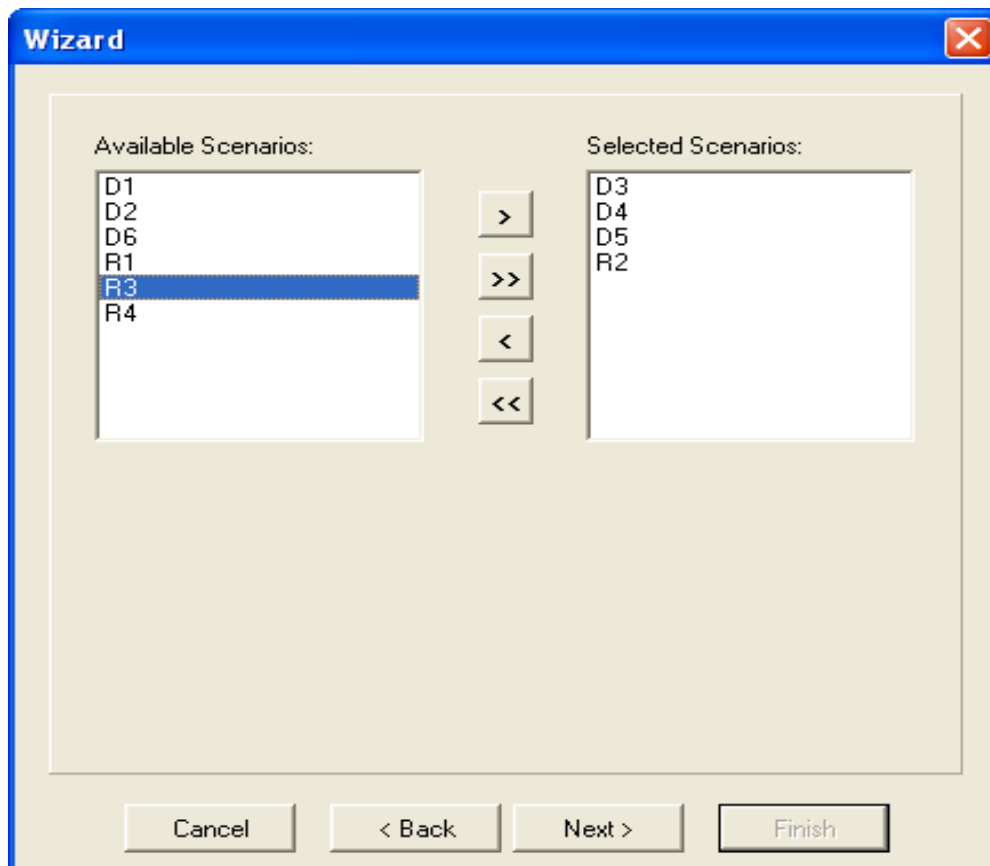

Figure 2.14: The User-Defined Wizard – Scenarios

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 (see Figure 2.15). On this form the user has to specify the name of the project and the description of the project. All SWASH output is put in a subdirectory of C:\SwashProjects. The SWASH output path can be changed by clicking on the button on the right-hand side of the 'path' field. Using the User-Defined wizard, the project name is set by default to [project_SubstanceName], but this can modified by the user. 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.
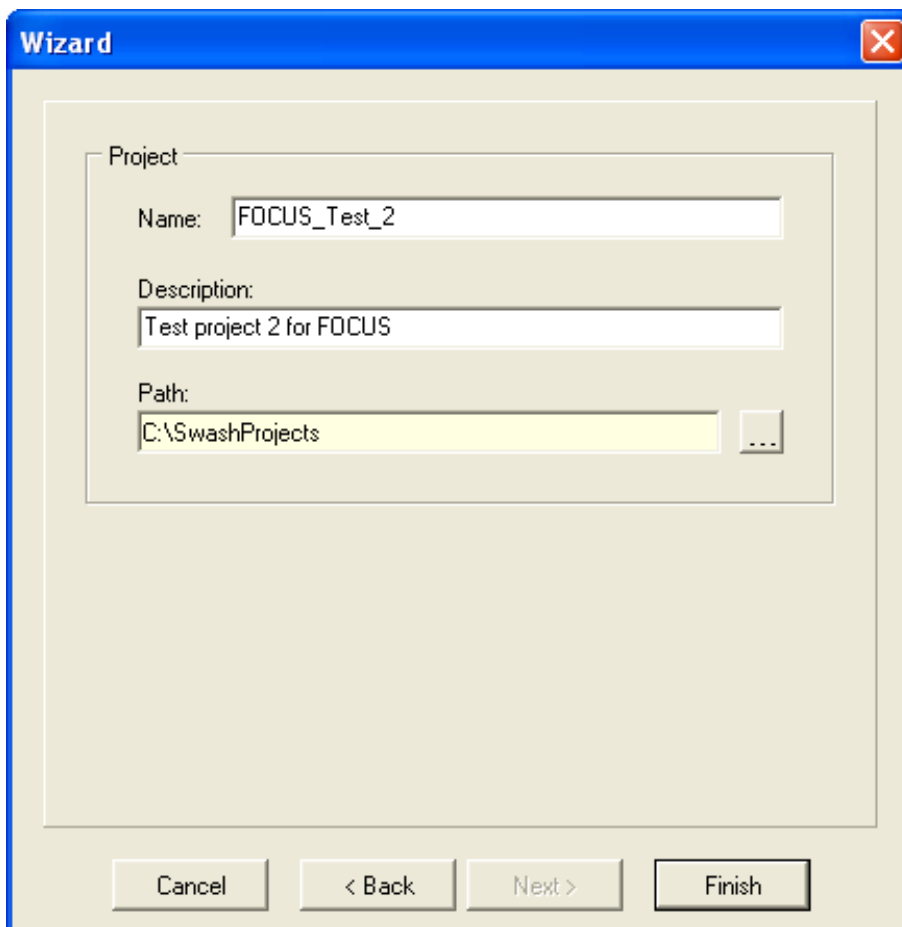
Figure 2.15: The User-Defined Wizard – Project Name and description

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 screen of SWASH.

2.1.4 View Projects and Define Applications

After clicking on the button 'View Projects and Define Applications' on the main screen, the form shown in Figure 2.16 is displayed on the screen (the example project from Section 2.1.2). The upper part is a browse part, where the user can browse through the list of available projects using the scroll bar on the right. For each project the most important elements are:
- The name of the project
- The description of the project
- The name of the substance.

In the lower part of the form the runs within the project selected are shown. The run information consists of the following:
- The runID: this a unique number; as MACRO or PRZM output can be used by TOXSWA for different water body types, an additional character is used to distinguish between the TOXSWA runs: p for Ponds, d for Ditch and s for Streams. The last three characters can be '_pa', '_m1' or '_m2', and these characters specify whether the fate of the parent compound is simulated in the run or metabolite 1 or metabolite 2.
- The crop

- The number of the crop within the season (the first or the second crop in the season)
- The scenario (see also Section 2.2.1)
- The water body type
- The number of applications
- Yes/No selected for report – by default set to Yes. If set to 'Yes' then the characteristics of the run are exported to a PRZM project file (przm.pzm) and the pesticide database of MACRO.

The user can select or unselect all runs for the report by clicking on the checkbox at the top right corner of the 'Runs' section of the 'Overview' form. For a specific selection, you can sort any column to get the right projects. The sorted column is marked with '*'
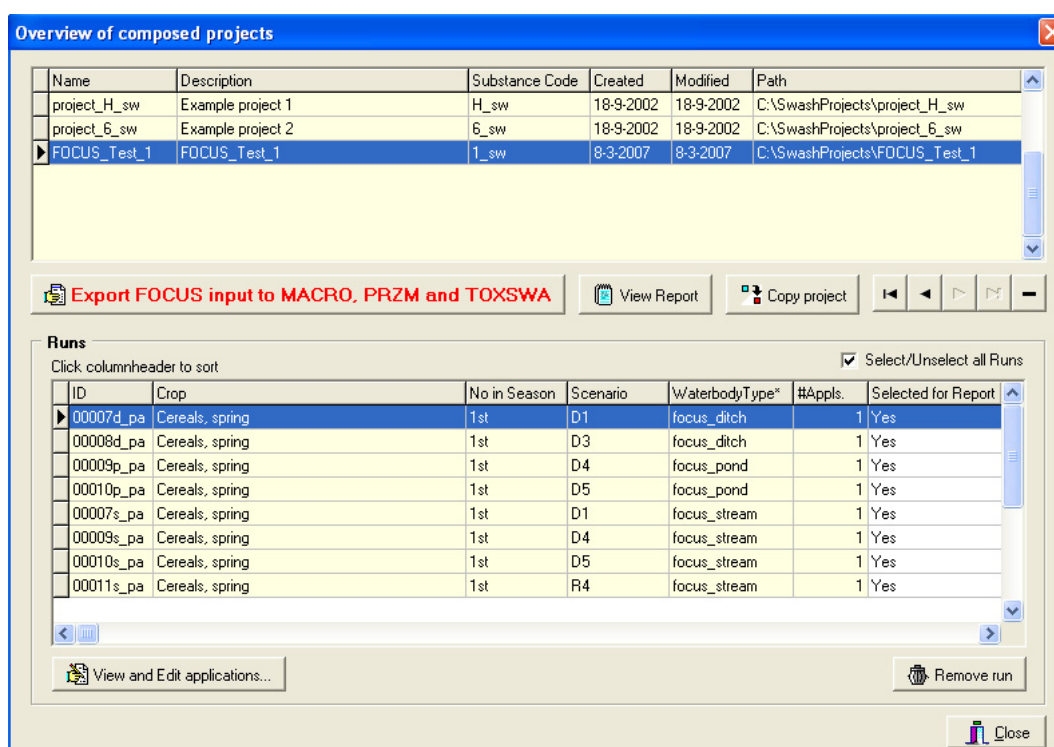
Figure 2.16: Overview of the FOCUS_Test_1 project created by the FOCUS wizard.

In Figure 2.17, only a part of the runs created by the User-Defined FOCUS wizard is shown. The other runs can be seen using the scroll bar on the right of the 'Runs' section of the 'Overview' screen.

Useful functionalities on the 'Overview of composed projects' screen are the buttons 'Copy project', 'View Report' and 'Remove run'. After clicking on 'Copy project' a copy will be made of the selected project, except that the project name and description are different. The user has to adjust those and then to edit the run specifications in the created project. Note that the values in the yellow boxes are fixed, so only the value for 'Selected for report' can be modified. After clicking on the 'Remove run' button a run is deleted. Note that a deleted runID number will not be used again in the SWASH database.

The 'Overview of composed projects' screen also contains a button 'View report'. By clicking 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.
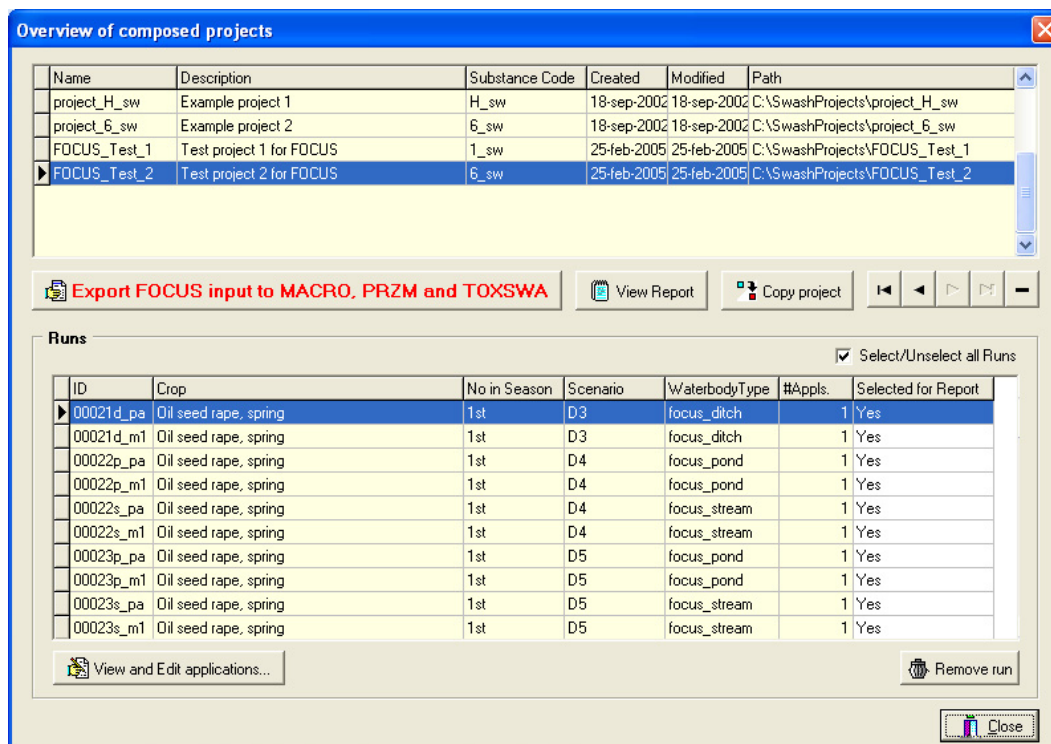
Figure 2.17: Overview of the runs in the FOCUS_Test_2 project created by the User-Defined wizard.

After clicking on the button 'View and Edit Applications' on the 'Overview of composed projects' screen, the form shown in Figure 2.18 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 these 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 is shown of available options (see Figure 2.18)
- 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
- The dosage (in kg ha^{-1})

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.

Default values used by SWASH are two weeks before emergence for the first possible day of application and 16 days after emergence for the last possible day of application. Thus, the period between the first and last possible day of application is 30 days.
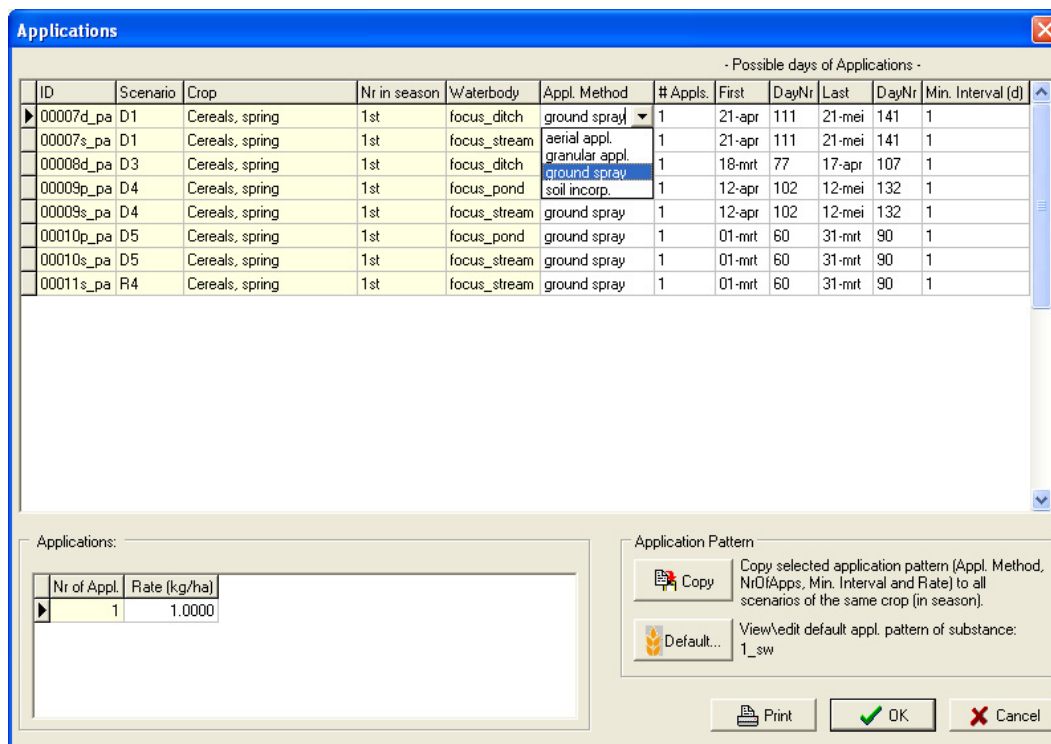
Figure 2.18: Application data for the runs in a project; a run for a Drainage scenario is selected

The input data on the application in the box in the lower-left part of the 'Applications' form as shown in the example shown in Figure 2.18 are input for a FOCUS run with a drainage scenario. Upon selection of a FOCUS run with a run-off scenario, e.g. the last run in the overview, the user has to enter a few more data to complete the run information. These input data are related to the method of application and are shown in Figure 2.19. The PRZM model has more options to introduce the substance in the soil, so the user has to specify in more detail the method of application. For more information on the application options for PRZM press F1 to enter the SWASH Help and then select 'CAM' (Chemical Application method). The overview of the runs can be printed by clicking on the 'Print' button.

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):

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

In which:
n   = number of applications
int   = minimum interval between two consecutive applications (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.
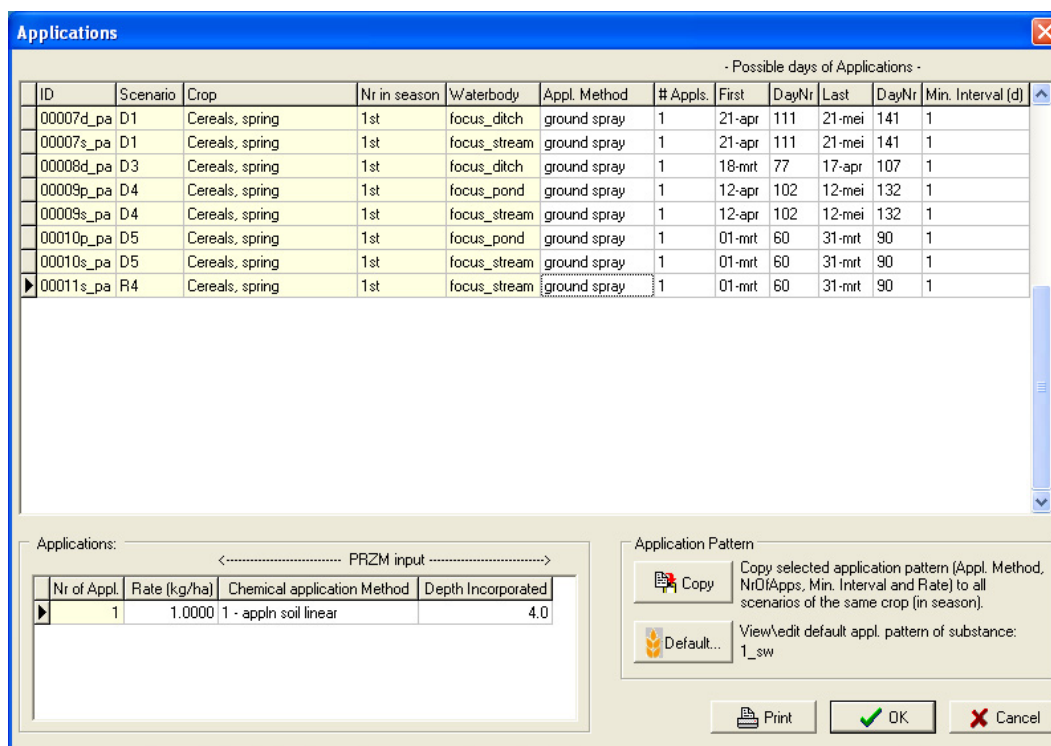
Figure 2.19: Application data for the runs in a project; a run for a Run-off scenario is selected.

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' screen, the user can enter default application patterns for a substance, that differ from the default SWASH defines. The form with data on the default applications is shown in Figure 2.20. The name of the substance the user has selected is displayed in the field at the top of the form. On this form the user can enter default values for a substance. The entries are:
- crop
- number of the crop within the year, i.e. is it the first or the second crop in the year

- scenario
- application method
- number of applications
- first day-in-year of application (Julian day number)
- last day-in-year of application (Julian day number)
- minimum time interval between two consecutive applications.

It should be noted that the dates in the date columns are adjusted automatically to the values entered for the day-in-year numbers.
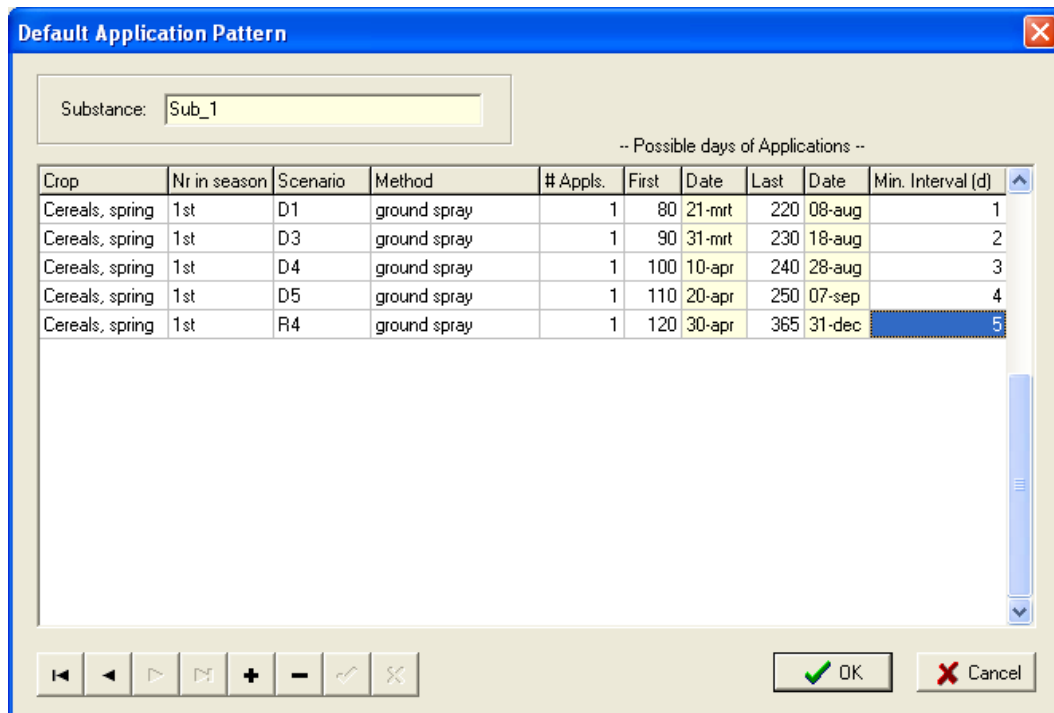
Figure 2.20. The substance form of SWASH – The default application pattern

The user should be aware that there is no check whether the application is within the crop period. If the period between the first day-in-year and the last day-in-year for the application is outside the cropping period, then the pesticide is applied to bare soil.

Once all input data have been entered correctly, the user returns to the 'Overview of composed projects' form 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. The options on the 'Create project files' form are shown in Figure 2.21. The user can select one or more options. After the appropriate options have been selected the user clicks on 'OK'.

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 screen 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.
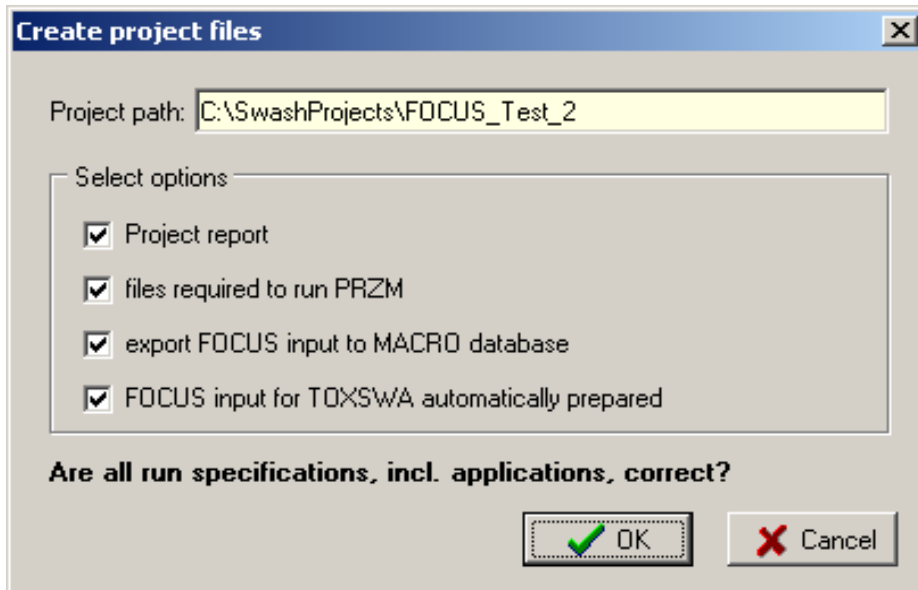
Figure 2.21: Create project files – options

2.1.5 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 screen 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). The main screen of the MACRO in FOCUS shell is shown in Fig. 2.22.
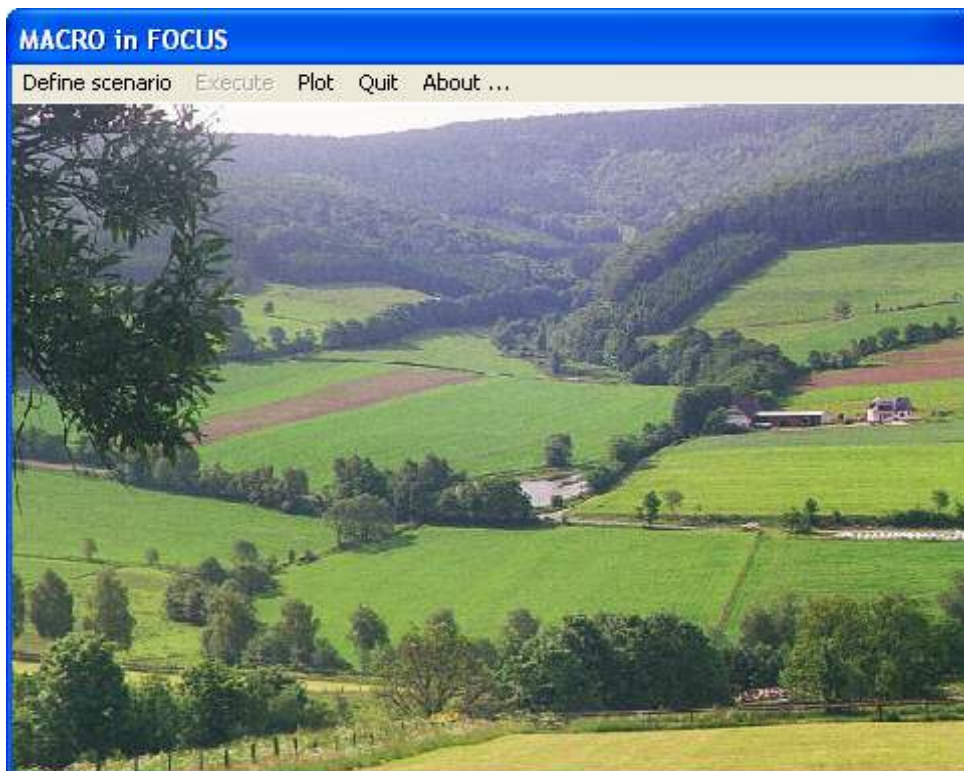
Figure 2.22 Main screen of MACRO in FOCUS

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 screen 'Define scenario' and then select 'Surface Water'.
- 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
- Select from the Menu bar at the top of the main screen 'Define' and then select 'parent compound'. The substance form is now shown (see Fig. 2.23).

Figure 2.23 Substance form of MACRO in FOCUS

- Select the substance for the run to be executed and confirm this by clicking on the button 'Select'; MACRO will return the message 'pesticide properties read from database'. Next click on 'OK'
- Select from the Menu bar at the top of the screen 'Define' and select 'Application'. Now the form presented in Fig. 2.24 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 'Run'. The PAT will give the message 'Solution found'. Then click on 'OK' and repeat this twice. The MACRO run is now fully defined: click on 'OK'.
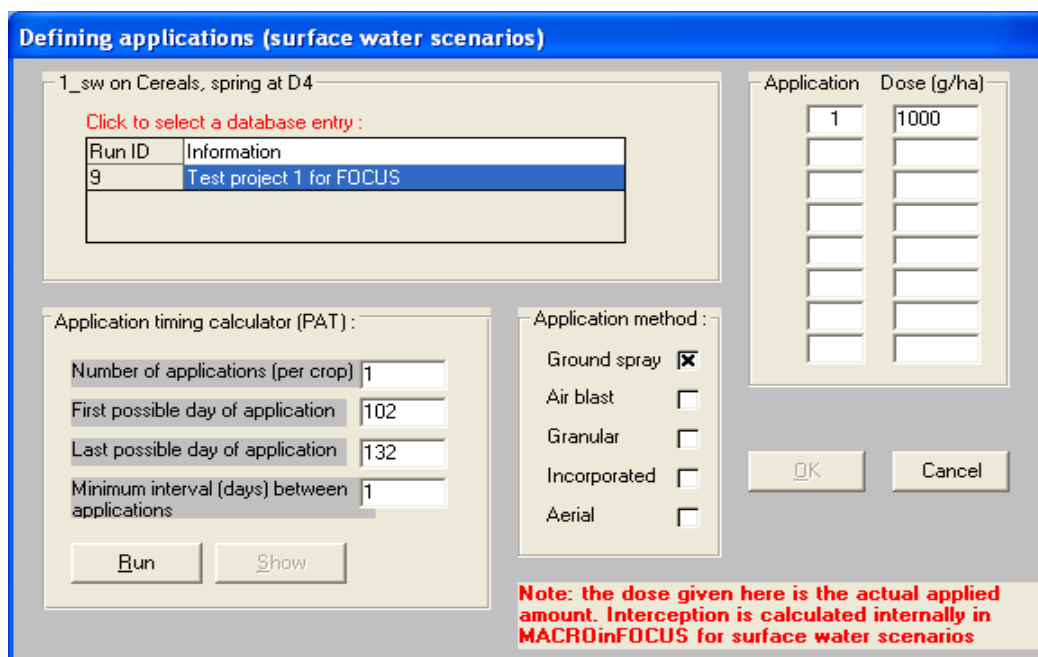
Figure 2.24 Application form of MACRO in FOCUS

- Select in the Menu bar 'Execute' and select 'current run'. 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 'Plot' in the menu of the main screen of MACRO. Now the form presented in Fig. 2.25 will be shown.
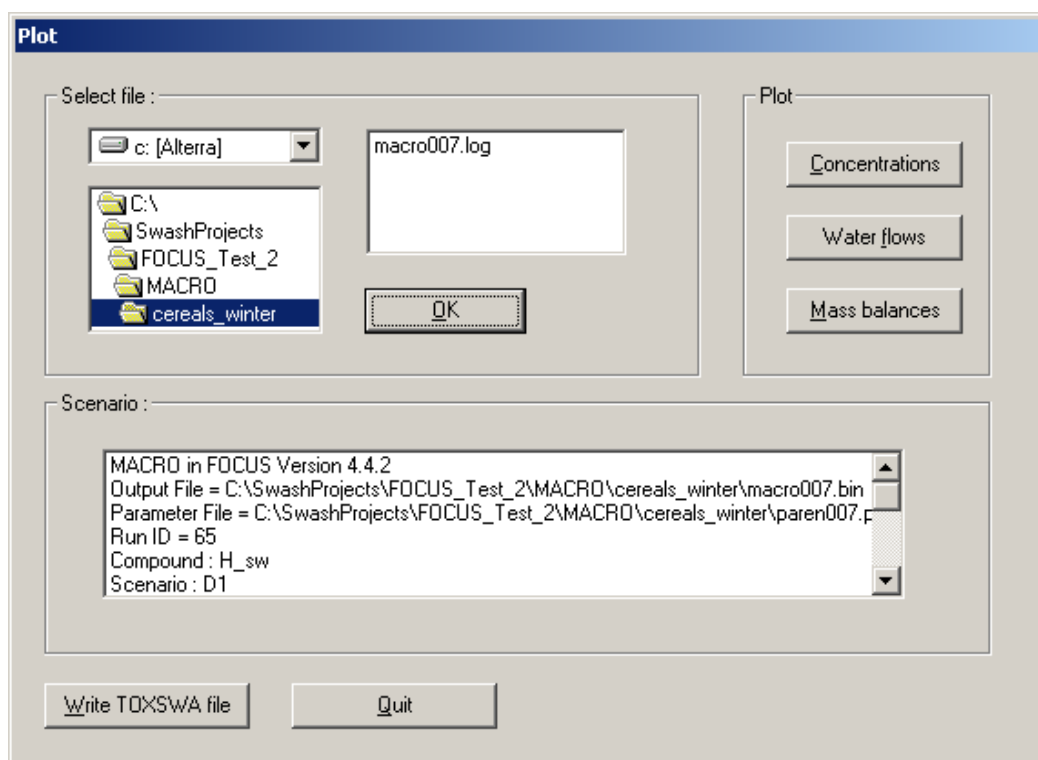
Figure 2.25 Creation of the MACRO output file with input to be read by TOXSWA

- 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 screen of MACRO.

2.1.6 Running PRZM

The user can start the PRZM shell by clicking on the 'PRZM' button on the main screen 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 screen of the PRZM shell is shown in Figure 2.26.

Figure 2.26 Main screen of FOCUS_PRZM

To start a FOCUS Surface Water run the following steps have to be done:
- Click on the button 'Import SWASH Project File'

Now the PRZM screen for selecting a SWASH projects will be shown; this screen is shown in Fig. 2.27.
- 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 2.26). 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.

Figure 2.27 SWASH Project screen of FOCUS_PRZM

2.1.7 Running TOXSWA

The user can start the TOXSWA shell by clicking on the 'TOXSWA' button on the main screen of SWASH. An updated version of the User's Manual for FOCUS TOXSWA has been published (Beltman *et al.*, 2006). In the following section only a short description on running FOCUS_TOXSWA_2_2_1 is given. The main screen of the TOXSWA GUI is now shown (Figure 2.28).

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

The following steps have to be done:
- Select the project containing the runs to be executed (see Figure 2.28).
- Open selected project by clicking on 'OK'
- Select the runs within the project by clicking on the field in the column 'Selected' to set the option at 'Yes' (see Figure 2.29).
- Click on the button 'Calculation'. Now the runs selected will be executed one after another.
- Click on 'Report' for each run executed to obtain the target data for the exposure assessment.
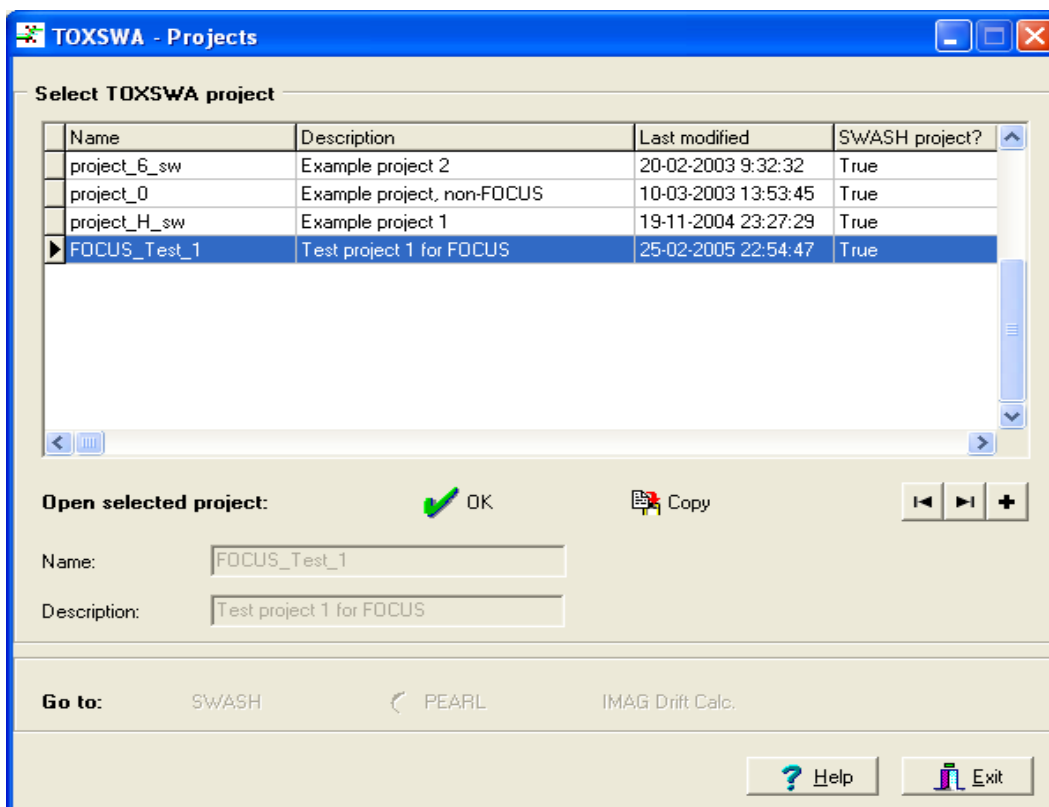
Figure 2.28 Project screen of FOCUS_TOXSWA
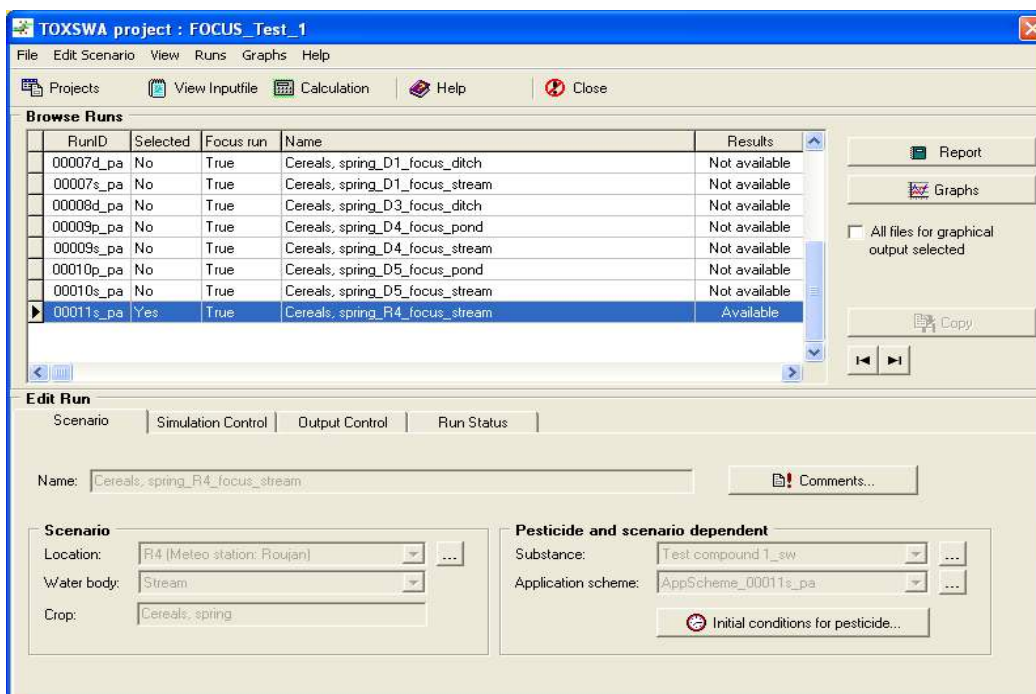
Figure 2.29 Project screen of FOCUS_TOXSWA

2.2   The Main Screen - Information

The main screen consists of two parts (see section 2.1). In the second part, 'Information', 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. The second part is displayed after clicking on the 'Information' tab and this is shown in Figure 2.30.
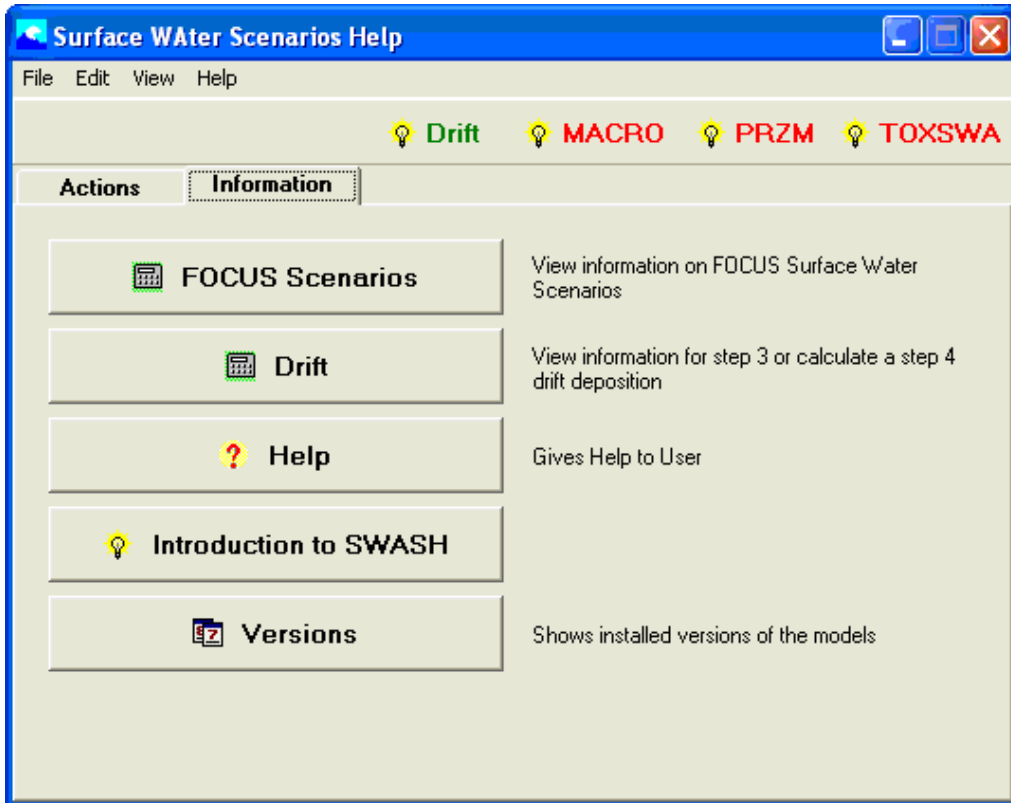
Figure 2.30: The main screen of the SWASH interface with the 'Information' tab displayed.

The 'Information' page of the main screen of SWASH contains five buttons. The function of the buttons will be briefly described here, but more detail 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 access to the Help function of SWASH. After clicking on this button, a list of items appears on the screen from which the user can select the item on which more information is required. Moreover, when using SWASH the user can get information on the form currently shown on the screen by pressing the F1 button on the key board. The Help function contains also a list of publications with more detailed information on specific subjects.

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 runs. The user is also explained that the separate models, MACRO, PRZM and TOXSWA still need to be run with the aid of their own shells, and how this proceeds.

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 workgroup. After clicking on this button, the 'FOCUS scenarios' page window presented in Figure 2.31 is shown on the screen. On this page three tabs with information are available. On the 'Crops' tab (see Figure 2.31) 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 occur are listed in the lower part of the form, as well as the emergence and harvest dates for each scenario.
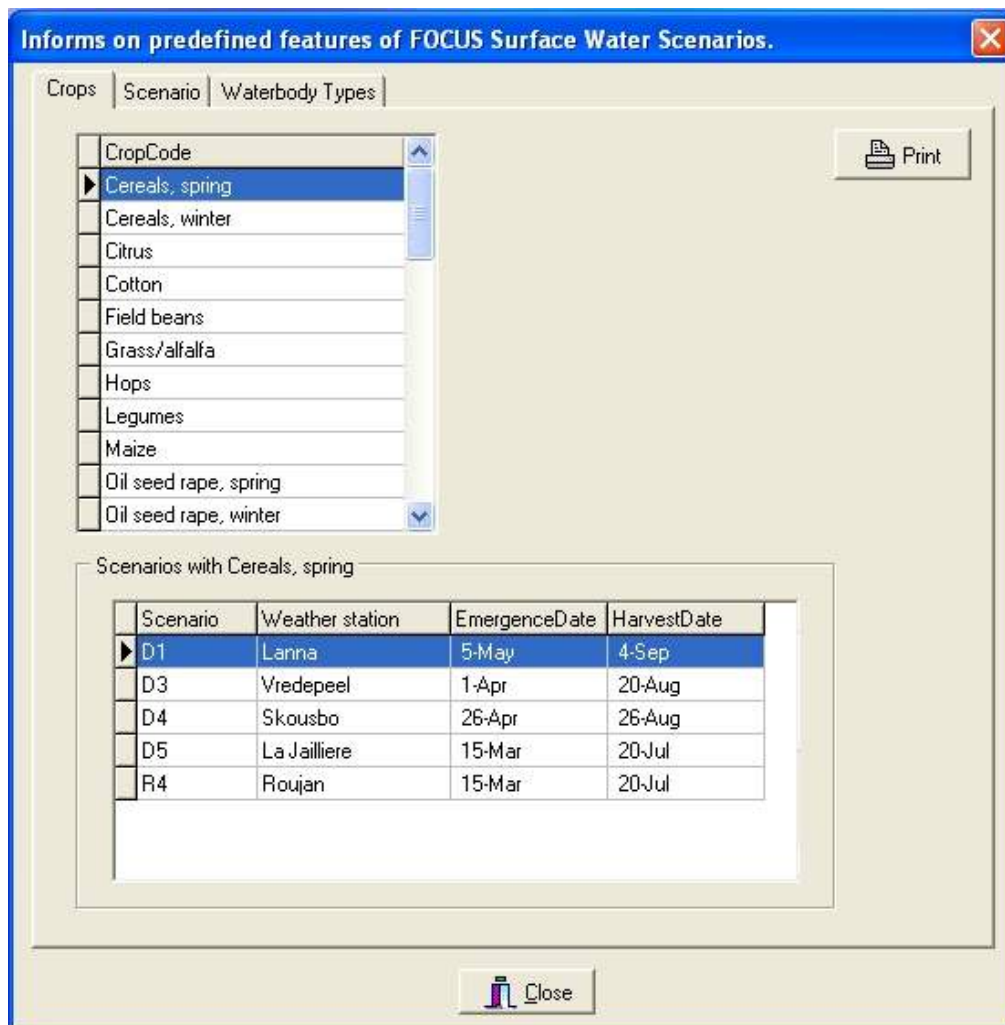
Figure 2.31: FOCUS Surface Water Scenarios – Crops.

On the 'Scenario' tab, as shown in Figure 2.32, the same information is presented differently from that on the 'Crops' page. On the 'Scenario' tab, 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 is 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 scenario selected is indicated.
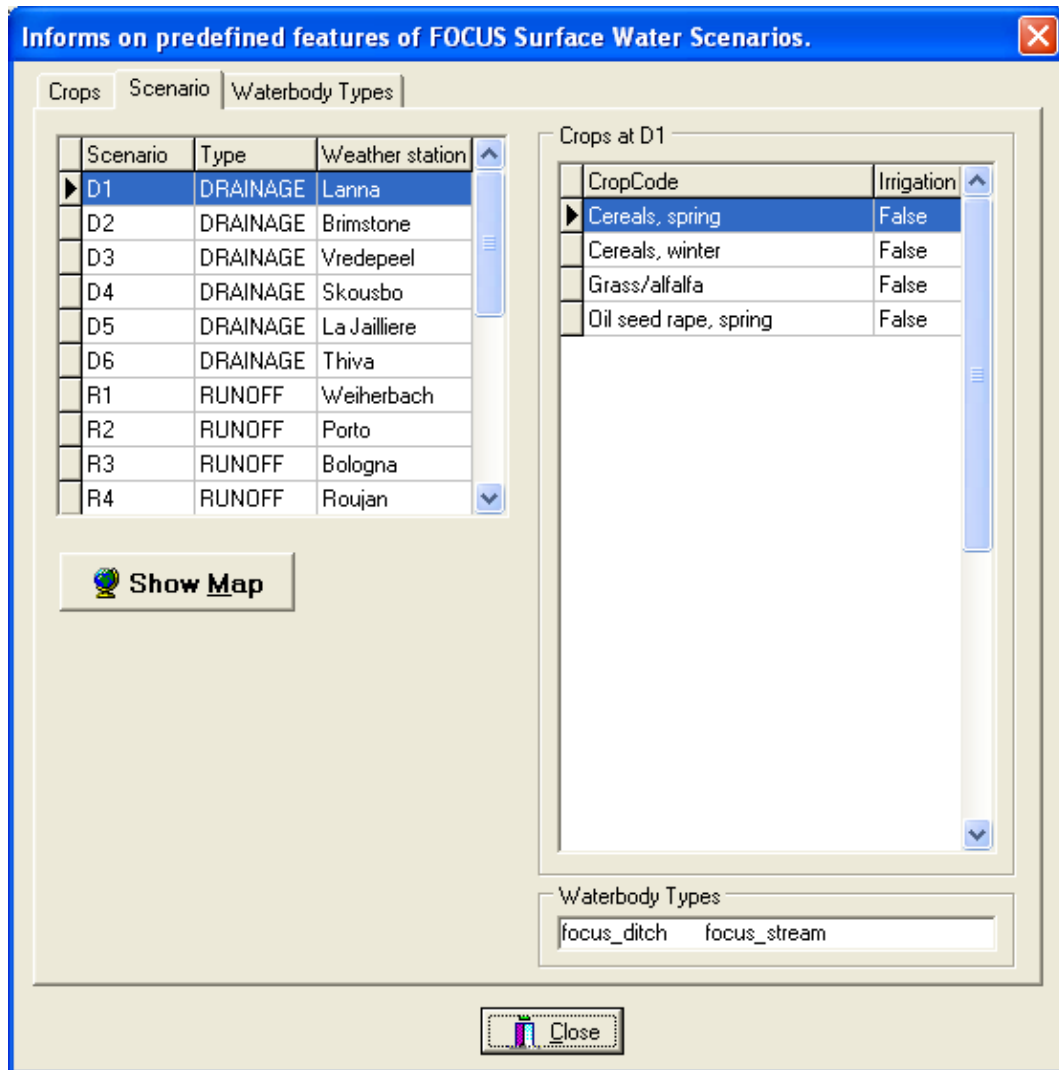
Figure 2.32: FOCUS Surface Water Scenarios – Scenario Types.

On the 'Water Body Types' tab, as shown in Figure 2.33, the user can get a list of available scenarios for a specific water body type. In the example present in Figure 2.33, the 'Ditch' Water Body Type is selected. In the set of FOCUS scenarios there are only 4 available scenarios (all drainage) for the FOCUS Ditch.
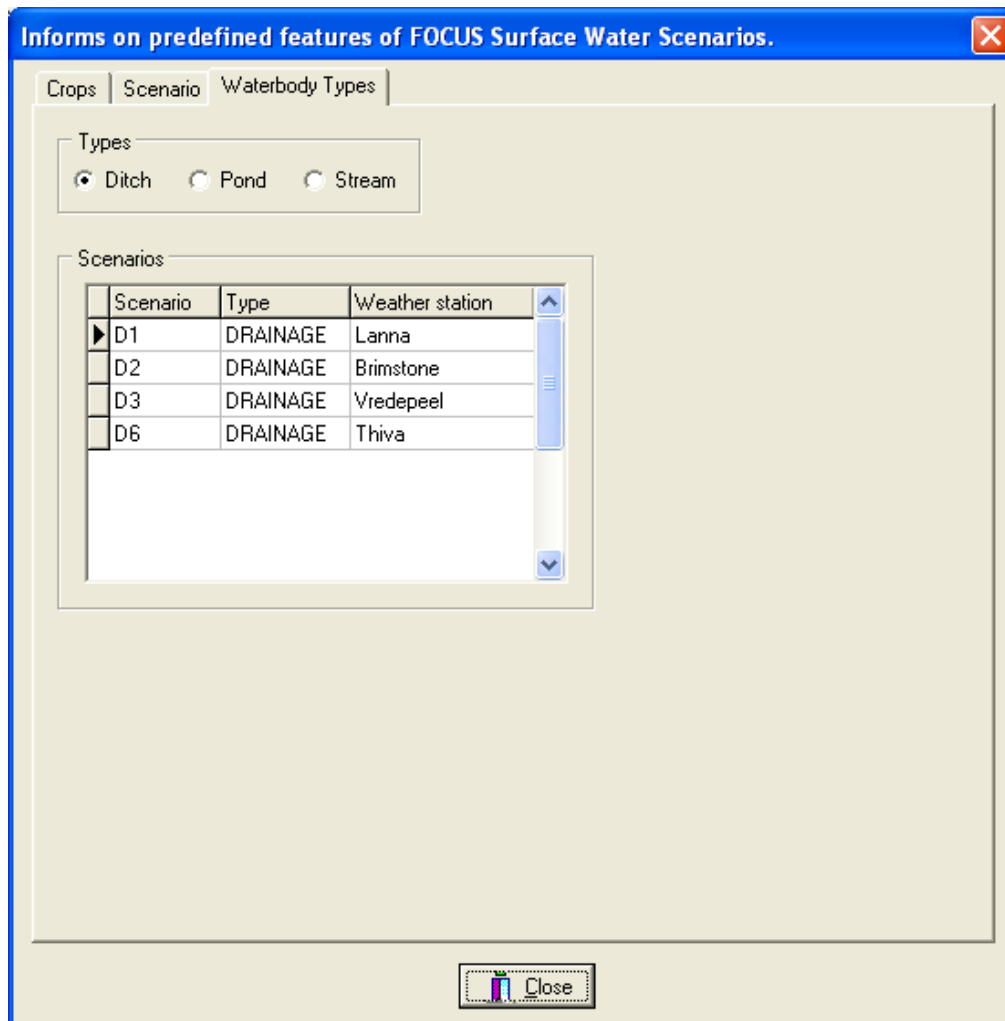
Figure 2.33: FOCUS Surface Water Scenarios – Water Body Types.

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 2.34 is shown on the screen. The user has to enter values for the fields 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 screen 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.

Figure 2.34: The FOCUS Drift Calculator

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.

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 a 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).

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.

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 screen. After clicking on 'Close' the user returns to the main screen of SWASH.

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_1.1.1 or FOCUS_TOXSWA_2.2.1. 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. Guidance on how to execute runs taking buffer zones into account is given in the User's manual of FOCUS_TOXSWA (Appendix L of FOCUS (2001) for version 1.1.1, Beltman *et al.* (2006) for version 2.2.1).

3 Installation and getting started

3.1 Installation

The SWASH software package can be downloaded from the FOCUS web site: http://viso.ei.jrc.it/focus/sw/index.html. The installation procedure results in the installation of SWASH_2.1. The installation directory is C:\SWASH by default. The MACRO, PRZM and TOXSWA software packages compatible with SWASH_2.1 should be installed in the same directory, i.e. C:\SWASH\MACRO, C:\SWASH\PRZM and C:\SWASH\TOXSWA respectively.
SWASH works only correctly if it is installed in the root of a harddrive. The driveletter maybe also another driveletter than C:.

FOCUS_SWASH_2.1 has been tested on Win2000, WinNT, WinXP and Vista. For WinNT a MS Office package is needed. SWASH is likely to run on previous versions, however, this has not been tested.

On WinNT, Win2000, WinXP and Vista machines it is necessary to have Administrator rights.

SWASH requires 12.5 Mb for installation. A monitor with at least a screen resolution of 800x600 is required, using 256 colours. Preferably, select 'small fonts' as display setting. The faster the processor the better.

The installation procedure for FOCUS_SWASH_2.1 depends on whether FOCUS_SWASH_1.1 has already been installed or not. The Read_me_first file that is supplied with the installation package contains the information for installation of FOCUS_SWASH_2.1

It should be noted that if FOCUS_SWASH_1.1 has already been installed then the user has the option to save the SWASH database and restore it when completing the installation of FOCUS_SWASH_2.1 (see Figure 3.1). Please note that the structure of the database in FOCUS_SWASH_2.1 is the same as that of FOCUS_SWASH_1.1. If the option 'save and restore database' has been selected, all user defined substances and projects will be saved.
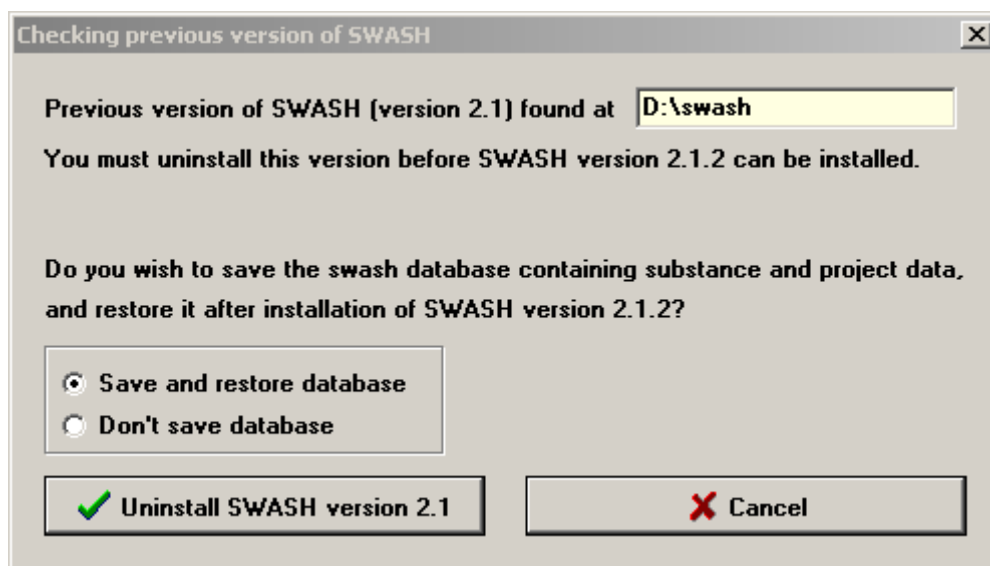
Figure 3.1 Installation options for previous installed FOCUS_SWASH

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 SWASH database or the creation of a new substance.

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

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, PRZM and TOXSWA shells.

This sequence of steps is depicted in Figure 3.2
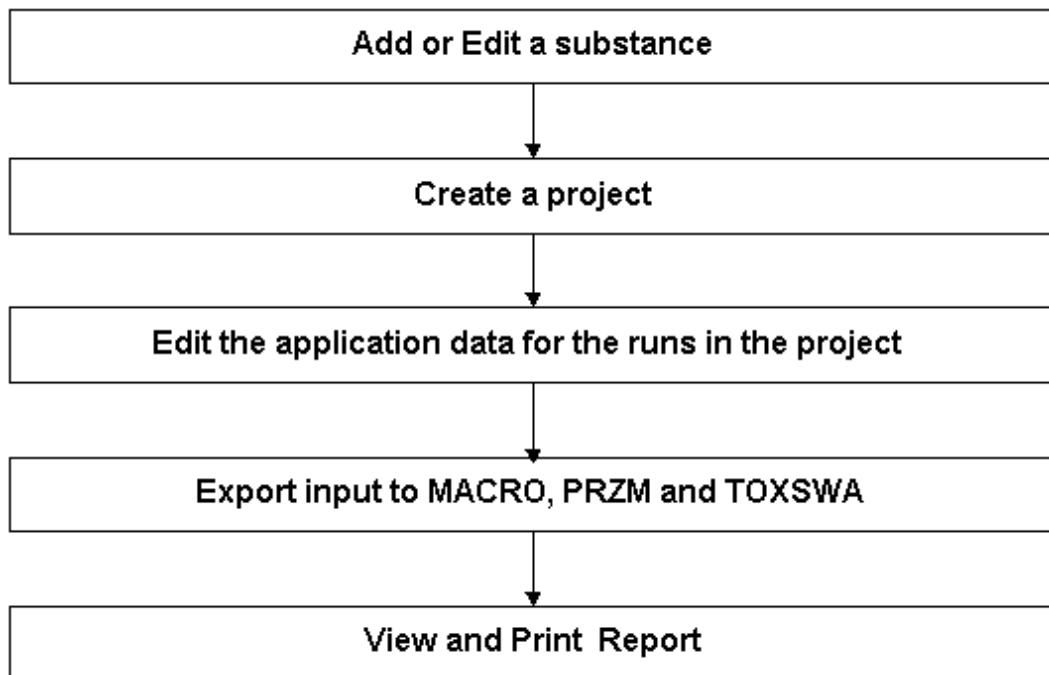
Figure 3.2 Scheme for preparing input to run FOCUS Surface Water Scenarios using SWASH.

Next runs have to be started in the sequence PRZM – TOXSWA or MACRO TOXSWA.

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 screen 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), and the

application scheme with the same runID as that for the corresponding run as defined in SWASH should be taken. After running MACRO the has 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 for TOXSWA.

The sequence of steps to specify and execute a drainage scenario for MACRO are also shown briefly in Figure 3.3.
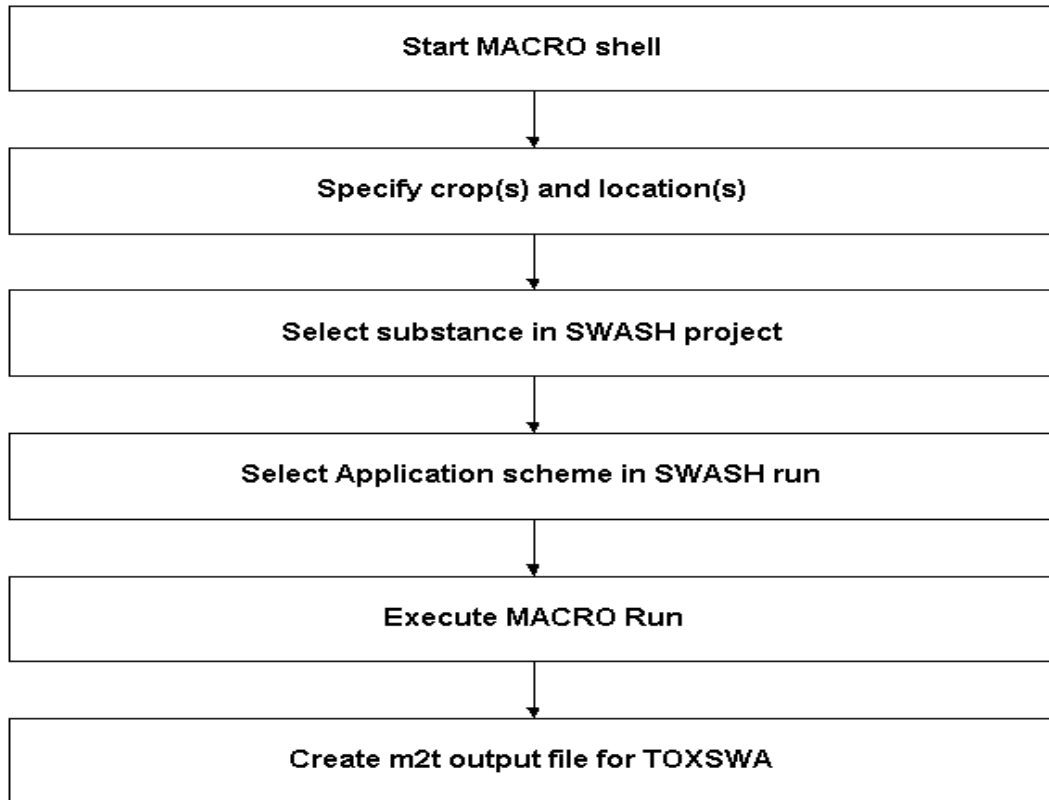
Figure 3.3 Scheme for executing a run with MACRO for a drainage scenario.

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 screen 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' screen. 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 3.4.
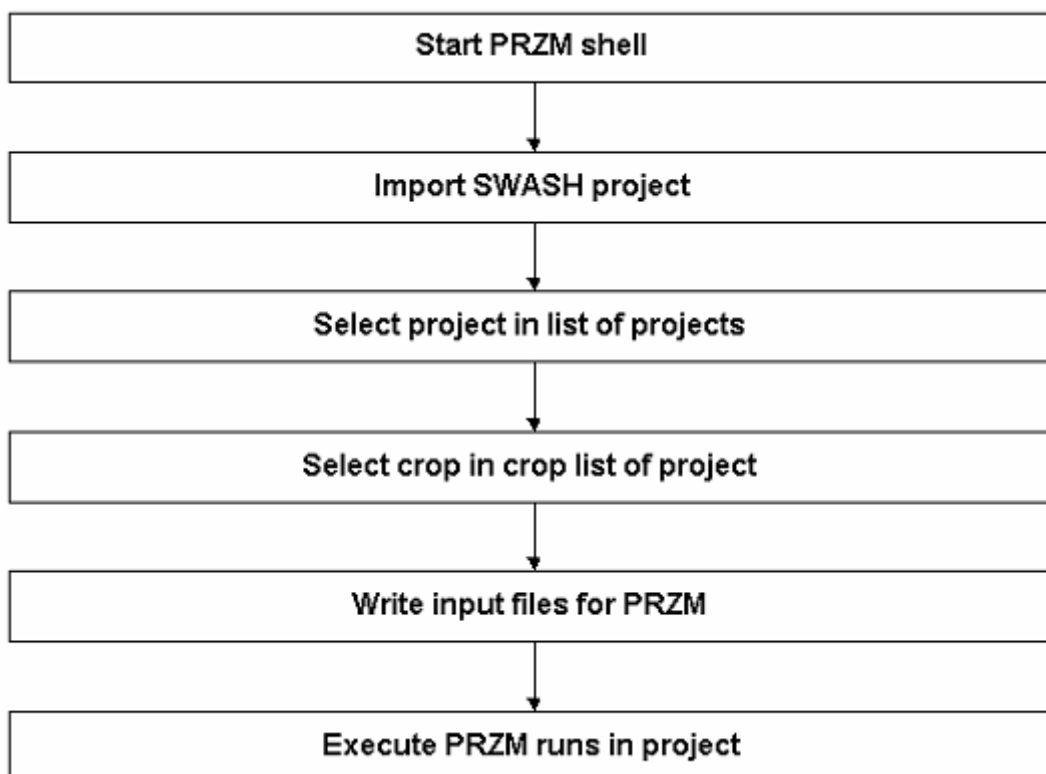
Figure 3.4 Scheme for executing a run with PRZM for a run-off scenario.

The last part of execution of a run for FOCUS Surface Water scenario is to run TOXSWA. The TOXSWA shell can be started after clicking of the 'TOXSWA' button. The steps to be followed are shown in Figure 3.5. It should be noted that 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.

Once the TOXSWA runs in the project have been completed, the user has the target data on the exposure concentrations (see TOXSWA's FOCUS reports).

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 do always an exposure assessment with TOXSWA for a single application with the highest application rate.

More detailed information on the TOXSWA model and guidance how to use FOCUS_TOXSWA is given in the User's manual of FOCUS_TOXSWA_2.2.1 (Beltman *et al.* ,2006).

Support for SWASH can be requested by sending an email to swash@pesticidemodels.eu.
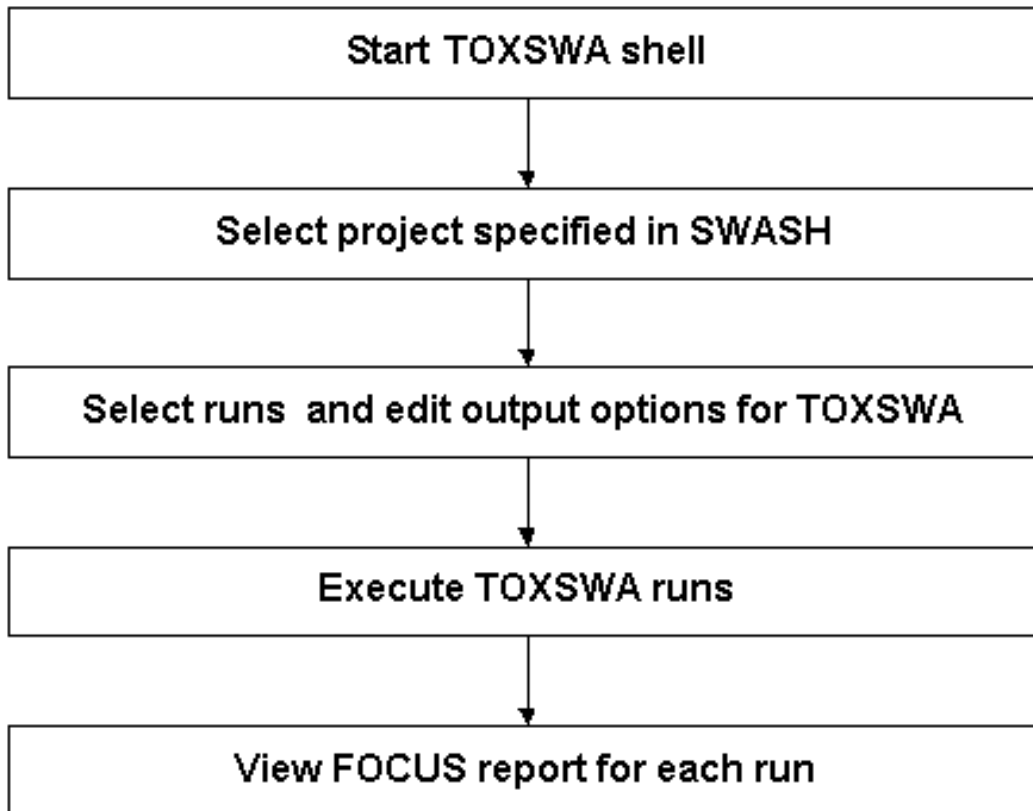
Figure 3.5 Scheme for executing a run with TOXSWA scenario.

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Annex 1 Example for creating a new substance in SWASH

To create a new substance the following steps have to be done:

1. Start SWASH

2. Press the button 'View and Edit Substances'. The 'Substances' screen is shown.

3. Press the button 'New' in the Substances screen. The 'New Substance' screen is shown.

4. Enter a unique code and name for the new substance you are going to define and click on the 'OK' button.

5. The 'Substances' screen appears again. You can now fill in the fields with data on the new substance. It should be noted that for some fields default values are given. These default values have been adopted in the Surface Water Scenarios.

6. Fill in the empty fields according to the table below.

Parameter	Value	Unit
Molar Mass	400	g/mol
Saturated vapour pressure	1 E^{-8}	Pa
Solubility in water	1	mg/L
Kom	600	L/kg
Koc	Koc is calculated by SWASH from Kom. Just click on the empty field and the value becomes visible	
DT50; Half life time water	300	d
DT50; Half life time soil	400	d
DT50; Half life time sediment	400	d
DT50; Half life time crop	1000	d

7. Click on the button 'View Metabolites' on the tab 'General'. Select the option 'One parent, no metabolite' and press the 'OK' button in order to return to the screen 'Substances'.

8. Press the button 'Save' in the screen 'Substances'. The substance you defined is saved in the database and is included in the list of substances.

9. Press the button 'Close' to return to the main screen of SWASH.

Annex 2 Example of a SWASH report

```
* SWASH report file
* made by FOCUS-SWASH UI v. 2 (= 2.1.2, 4 Dec 2007)
*
* File Name   : C:\SwashProjects\project_6_sw\project_6_sw_report.txt
* Description : Example project 2
* Substance   : Test compound 6_sw
*
* Creation    : 05-mrt-2008, 09:55
*
* 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
*
*            N.B. 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.
```

Fig A2-1 The header of the SWASH report.

```
*************************************************************************************************************
*   CREATED RUNS
*************************************************************************************************************
*
*                                                         |--------------- APPLICATION ----------------|----- on Water Surface -----|
* --ID--MACRO\PRZM-Crop(1st/2nd)----------Scenario-WaterbodyType-|-Method---------First/Last/Interval-#--Rate-|-Mean Deposition-Mass Loading
*                                                                                           (d)        (kg/ha) (% of Appl. Rate)    (mg/m2)
*
* 00004p_pa 00004  Cereals, winter(1st)    D4        focus_pond   ground spray   08-sep/28-okt/7    1 1.0000       0.154            0.154
*                                                                                                   2 0.7500       0.154            0.116
*                                                                                                   3 0.5000       0.154            0.077
*
* 00004p_m1 00004  Cereals, winter(1st)    D4        focus_pond   ground spray   08-sep/28-okt/7    1 1.0000       0.154            0.154
*                                                                                                   2 0.7500       0.154            0.116
*                                                                                                   3 0.5000       0.154            0.077
*
* 00005d_pa 00005  Cereals, winter(1st)    D6        focus_ditch  ground spray   16-nov/16-dec/1    1 1.0000       1.927            1.927
*
* 00005d_m1 00005  Cereals, winter(1st)    D6        focus_ditch  ground spray   16-nov/16-dec/1    1 1.0000       1.927            1.927
*
* 00006s_pa 00006  Cereals, winter(1st)    R1        focus_stream ground spray   29-okt/29-nov/1    1 1.0000       1.716            1.716
*
* 00006s_m1 00006  Cereals, winter(1st)    R1        focus_stream ground spray   29-okt/29-nov/1    1 1.0000       1.716            1.716
*
**************************
************************** Surface WAter Scenarios Help *********************************************************
```

Fig A2-2 The Created Runs section of the SWASH report

Annex 3 Day in year calendar

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

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