

Surface WAter Scenario Help (SWASH) version 1.94

Confinanced by ECPA and DG SANCO

Surface Water Scenario Help (SWASH) version 1.94

Technical Report version 1.3

**J. A. te Roller
F. van den Berg
P.I. Adriaanse**

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ABSTRACT

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The user-friendly shell SWASH, acronym for Surface Water Scenarios Help, assists the user in calculating pesticide exposure concentrations in the EU FOCUS surface water scenarios. SWASH encompasses four separate tools and models: (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 maintains a central database with pesticide properties and also information on projects and runs created by the user. This report gives a detailed description of the necessary flow of data between the various models, to make them communicate smoothly with each other. It also specifies the installation requirements for the MACRO, PRZM and TOXSWA models. The MACRO model uses an MS-Access database to store its substance and run information, while PRZM makes use of separate data files. TOXSWA uses the central SWASH database. After completing a SWASH session the user should manually perform simulations with the three individual models.

Keywords: FOCUS, MACRO, Pesticide, PRZM, Scenario, Surface Water, TOXSWA, Substance, Installation, Database, User-friendly Shell, Software Development.

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P.O. Box 47, NL-6700 AA Wageningen (The Netherlands).
Phone: +31 317 474700; fax: +31 317 419000; e-mail: postkamer@alterra.wag-ur.nl

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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, that will be used for aquatic risk assessment in the pesticide registration procedure at EU level. In the proposed Step 3 calculations several tools and models need to be combined to calculate exposure concentrations in the various types of surface water bodies. To promote an easy and consistent way of calculation the idea rose to develop an overall user-friendly software shell 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 end 2002 SWASH, acronym for Surface Water Scenarios Help, was developed by Erik van den Berg and Paulien Adriaanse from Alterra, in cooperation with Daniel van Kraalingen and Johnny te Roller from WISL (Wageningen Software Labs). 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, 2002) and this instrument has also been included in SWASH.

SWASH has been financed by various sources. In 2000 the ECPA (European Crop Protection Agency) procured 20 keuro, and the Dutch Ministry for Agriculture, Fisheries and Nature Management also allocated 41 kf (about 19 keuro) for SWASH. In 2001 DG SanCO from the EU contributed 38 keuro and in 2002 the Dutch Ministry for Agriculture, Fisheries and Nature Management financed the remaining 20 keuro to finalise SWASH.

The current document (Alterra rapport 508) is a technical document, explaining the technical design of the SWASH database and communication and installation procedures. This document will be helpful for possible, future extensions or updates.

Additionally an user's manual has been written (F. van den Berg et al, 2002). This is intended to explain to users how to use SWASH and next, perform the Step 3 FOCUS Surface Water Scenarios runs.

At present (SWASH version 1.9) the coupling SWASH-PRZM has not yet been extensively tested. This implies that specifications with respect to the PRZM model may change in the next version of this document.

Summary

To carry out the EU FOCUS pesticide exposure assessment scenarios for surface waters, a number of FOCUS tools and models have to be run in sequence. Each of these tools and models have been developed separately targeting a specific aspect relevant to the assessment. These are:

- Drift Calculator, calculating pesticide transport through drift
- PRZM-3, calculating pesticide transport through run-off
- MACRO, calculating pesticide transport through drainage
- TOXSWA, 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 a number of individual tools and models involved in Step 3 calculations.

The pesticide transport through drift is automatically calculated by the Drift Calculator. The Drift Calculator can be also used as a tool to calculate spray drift depositions for separate, not standard FOCUS step 3, runs.

PRZM-3 is a model that uses binary files to store information on substances. These files are updated by SWASH.

MACRO is a run-oriented model. It uses a MSAccess database (pest_focus.mdb) to store information on substances and runs. This database is updated by SWASH.

SWASH is project-oriented. The user defines a project for a substance. In the project runs are created for the selected crops, scenarios and waterbody types. For each project SWASH can generate a report with an overview of all the runs.

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

Finally, SWASH proposes a directory structure for the various models and their input and output to enable a smooth and correct communication between the various tools.

After completing a SWASH session, the user must manually perform simulations with the individual models: PRZM, MACRO and TOXSWA. From SWASH it is possible to start the shells of these models and perform the simulations. SWASH prepared the models to guide the user easily through the various runs 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 the EU FOCUS pesticide exposure assessment scenarios for surface waters, a number of FOCUS tools and models have to be run in sequence. Each of these tools and models have been developed separately targeting a specific aspect relevant to the assessment. These are (between brackets the name of the contact person for each tool has been mentioned):

- Drift Calculator, calculating pesticide transport through drift (M. Russell)
- PRZM-3, calculating pesticide transport through runoff (M. Russell)
- MACRO, calculating pesticide transport through drainage (N. Jarvis)
- TOXSWA, calculating the fate of pesticides in surface waters (P. Adriaanse)

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 a number of individual tools and models involved in Step 3 calculations. The main functions of SWASH are:

- Maintenance of a central pesticide properties database. Updating MACRO database (pest_focus.mdb) and PRZM data-files (chmdat.dat, chmnum.dat),
- Provision of an overview of all Step 3 FOCUS runs required for use of a specific pesticide on a specific crop. Therefore a project is created containing all needed runs with unique runId's for all models.
- Calculation of spray drift deposition onto various receiving water bodies and
- Preparation of input for the MACRO, PRZM and TOXSWA models. Exporting run information to the MACRO database. Creating a przm.prj file with run information for PRZM. Updating the SWASH database to prepare for TOXSWA.

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

Finally, SWASH proposes and creates a directory structure for the various models and their input and output to enable a smooth and correct communication between the various tools.

After defining a project in SWASH the user can start from SWASH the other 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.

2 Dataflow between the models

SWASH is responsible for the flow of data between the models. Figure 2.1 shows a scheme of the dataflow.

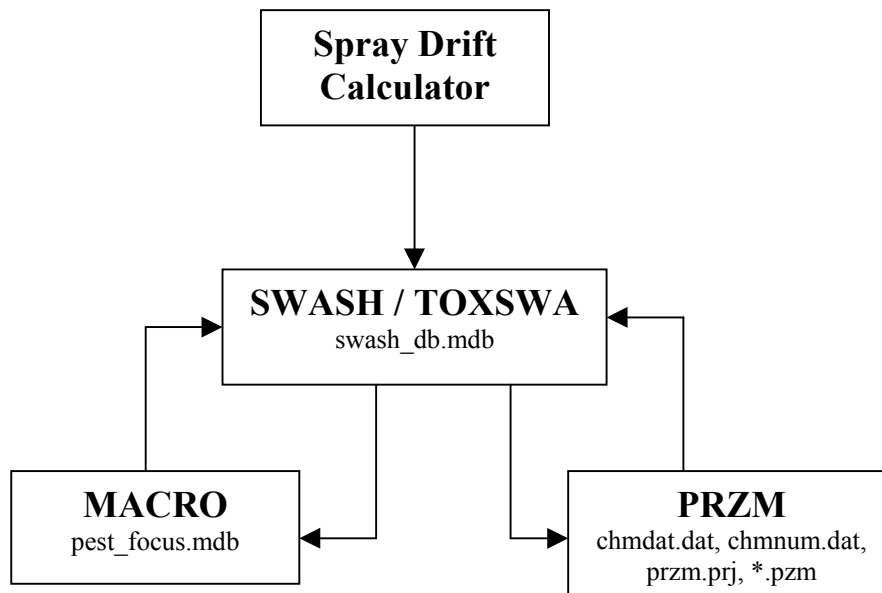


Figure 2.1 Flow of data between the models

SWASH gets input from the Drift Calculator. The drift percentage is calculated and used by SWASH as input for TOXSWA.

TOXSWA uses the same database as SWASH. No transfer of data is necessary. SWASH just updates some tables in the database that are used by TOXSWA.

SWASH updates the database of MACRO with information of the pesticides. Pesticides created by MACRO are transferred back to SWASH. Runs created in a SWASH project are exported to MACRO. It is not possible to create runs in MACRO so no run information has to be exported from MACRO to SWASH.

SWASH updates the data files chmdat.dat and chmnum.dat of PRZM with information of the pesticides. Pesticides created by PRZM are transferred back to SWASH. Projects created by SWASH are stored in the file przm.prj. This file is used by PRMZ to locate the information of the runs in the projects. Information of the runs needed for one crop is stored in pzm-files.

3 Data Structure

The central pesticide database (SWASH database) stores information on physico-chemical properties as well as the use patterns of the compound. Data can be entered directly by the user using the SWASH shell or data can be uploaded from the chemical property databases of MACRO or PRZM. After exiting SWASH (or choosing to update the database during a SWASH session), the information in the central database is written back into the databases of MACRO or in sets of input files for PRZM. TOXSWA makes use of the SWASH database. In this way SWASH ensures that identical or consistent information on pesticide properties and pesticide use is introduced into the consecutive model runs.

The database holds, among other data, information about crops, locations, occurrence of crops in locations, pesticide properties, use patterns of chemicals on crops and water body types of locations (i.e. pond, ditch, stream).

The SWASH application communicates with the database and interacts with the user on the type of assessment to be made. The application allows the user to select a chemical, a crop and a use pattern.

3.1 SWASH database

See Appendix 1 for the database structure of the SWASH database. It is located at the \SWASH\DATA directory.

3.1.1 Projects

In SWASH the user creates projects. Each project is characterised by one substance (table *projects*). Therefore it has a link to the *substances* table with all the information about the substance.

Each project has one or more runs (table *runs*). This means for one substance several runs can be defined. Each run is characterised by a location, crop and waterbody type and has a specified application scheme (table *applications*).

3.1.2 Runs

In SWASH each run is characterised by a unique run identity number (runid). The SWASH runid has the format *12345w_pm*, in which:

12345	a unique 5-digit number, enabling a maximum of 99999 different runs to be distinguished
w	water body type: p = pond, s = stream and d = ditch
pm	substance type: pa = parent, m1 = metabolite 1 and

m2 = metabolite 2.

So, a run id of 00010d_pa indicates run number 10 and relates to a parent substance in a ditch.

The TOXSWA model uses exactly the same runids as SWASH does.

However MACRO has another system to number runs and does not need to distinguish between different water bodies. Its input files and output files have names according to the format *names123.ext*, in which:

names	specifies file name: macro, paren or metab
123	a unique 3-digit number, enabling a maximum of 999 different runs to be distinguished
ext	specifies file extension, e.g. .par, .bin, .log, or .sum.

Only the m2t output file, containing the water and pesticide fluxes entering the waterbody, is named differently. This output file has the format Macro12345_x.m2t, in which:

Macro	specifies file name
12345	the unique 5-digit number, corresponding with the SWASH runid for the indicated run. N.B. Note that this 5-digit runid differs from the 3-digit runid of MACRO !
x	Substance type: p = parent, m = metabolite. MACRO can only handle one metabolite per parent run
m2t	extension, indicating this the MACRO output file with lateral entry fluxes for TOXSWA.

The PRZM model does not use run identity numbers to identify input files and output files, except the p2t file, containing the water and pesticide fluxes for TOXSWA. Like MACRO it does not need to be able to distinguish between the different water body types. The p2t output file has the format *12345_Cx.p2t*, in which:

12345	the unique 5-digit number, corresponding with the SWASH runid for the indicated run.
Cx	Substance type: C1 = parent, C2 = first metabolite and C2 = second metabolite (parallel or consecutively formed) PRZM can handle both metabolites in a single run.
p2t	extension, indicating this the PRZM output file with lateral entry fluxes for TOXSWA.

More details on the run identity numbering are given in the first section of Chapter 4.

3.1.3 Substances

A user can use default FOCUS substances but more likely he will use his own defined substance. Information about the substances is located at the tables *substances*,

substance_Macro and *substance_PRZM*. Table *substance_Macro* contains information specific for the MACRO model. *Substance_PRZM* contains information specific for the PRZM model.

3.1.4 Global information

Data for projects and substances can be changed by the user. Next to these data the database contains static data that is used by SWASH and contains information about crops, locations, occurrence of crops in locations, pesticide properties, use patterns of chemicals on crops and water body types of locations (i.e. pond, ditch, stream). The user can just view this information. e.g. a list with crops for a specified scenario.

The tables *substancexcropxlocation* and *cropsxlocations* store some default values on the application pattern.

The tables *Waterbodies*, *Ganzelmeier* and *Regression* have data needed for the drift calculator.

3.2 MACRO

MACRO uses three MSAccess databases:

1. *crops.mdb* : crop information
2. *focus.mdb* : soil information
3. *pest_focus.mdb* : run and substance information

SWASH only uses the *pest_focus.mdb*. Appendix 2 shows the structure of this database. It is located at the main MACRO directory, \SWASH\MACRO.

The tables *compound* and *metab* have the substance information where as the tables *run* and *applications* hold the project information. However MACRO doesn't define projects but just uses runs. Each run is characterised by a substance (compound), location and crop.

3.3 PRZM

PRZM stores its information in data files. The files *cbmdat.dat* and *cbmnum.dat* are used by SWASH. These files contain the substance information, *cbmdat.dat* the real information and *cbmnum.dat* the number of substances. They are located at the subdirectory \SWASH\PRZM\WPIC.

3.4 TOXSWA

TOXSWA uses the same database as SWASH. In SWASH a project can contain just one substance. In TOXSWA one project can contain several substances. Therefore some extra tables are added to the SWASH database: *Toxswamap* and *MapxProject*. A Toxswa-map exists of one or more SWASH-projects. So a TOXSWA-map can contain one or more substances.

TOXSWA runs are linked to a Application scheme. This scheme has one or more applications and can be used by one or more runs. In SWASH each runs has its own applications.

These two points make it necessary that SWASH prepares the database for TOXSWA.

3.5 Matching Data

At the start of SWASH, runs and substances are imported from the MACRO database and substances from PRZM. PRZM doesn't store information of runs or projects.

At the end of a SWASH session substances are exported to the MACRO database and to the PRZM files.

When the user in SWASH has created a project and has selected the option to export FOCUS input, runs are exported to the MACRO database. This option also creates input files for PRZM.

Before the user starts the MACRO shell from SWASH runs and substances are exported to the MACRO database. When the user quits MACRO and returns to SWASH substances created during the MACRO session are imported into the SWASH database.

Analogously, run and substance information is exported to the PRZM data files przm.pzm and chmdat.dat, chmnum.dat, when the user starts the PRZM shell. When the user quits PRZM and returns to SWASH substances created during the PRZM session are imported in the SWASH database.

TOXWA uses the SWASH database therefore no further matching of data for TOXSWA is necessary.

3.5.1 Export runs to MACRO

With the 'Export FOCUS input to MACRO, PRZM and TOXSWA' button in SWASH all runs are exported to the MACRO database. This means adding or replacing the records in the *runs* and *applications* tables.

Just one run is created in MACRO for locations with more than one waterbody type.

These are the matching fields in the MACRO and SWASH tables.

MACRO

run:

- runid (i.e. communal
SWASH runID)
- first_day
- last_day
- num_apps
- min_int
- app_method

SWASH

Runs:

- RunID (without s,p,d and pa,m1,m2)
- FirstDayYrApp
- LastDayYrApp
- NumberOfApps
- MinIntervalApps
- AppMeth

- compound	Projects.SubstanceCode
- cropname	- CropCode
- location	- LocationCode
- text_info	Projects.Description
- PathInOut	Projects.Path + '\MACRO\' + CropCode (without illegal characters like space and &,*?)
- projectname	Projects.Name
- projectid	Projects.ID

applications:	Applications:
- RunID	- RunID (without s,p,d and pa,m1,m2)
- ApplicationNr	- ApplicationNr
- Dose	- Rate

3.5.2 Import substances from MACRO

At the beginning of SWASH or when the user returns from the MACRO shell to SWASH, all substances (table *compound* and *metab*) are imported from the MACRO database. New substances are added and the others are updated. Default SWASH has some FOCUS substances. These are read only and can not be changed. The field *Locked* is set to true.

These are the matching table fields. If there is no matching field SWASH creates default values. (Table names in bold).

<u>SWASH</u>	<u>defaults</u>	<u>MACRO</u>
compounds		
substances:		compound:
<i>for new substances:</i>		
- SubstanceCode		- name
- IsParent	true	
- Locked	false	
<i>for all substances if not locked</i>		
- Name		- inform
- ExpFre		- freund
- Kom		- koc/1.724
substance_Macro:		
- inform		- inform
- Koc		- Koc
- halflife		- halflife
- tref		- tref
- vap		- vap
- VpTemp		- VpTemp
- pf		- pf

- expb
- tresp
- freund
- diffusion
- fstar
- fext
- candeg

- expb
- tresp
- freund
- diffusion * 86400
- fstar
- fext * 1000
- candeg

metabolites

substances:

for new substances:

- SubstanceCode
- IsParent false
- Name
- Locked false

for all substances if not locked

- Name
- ExpFre
- Kom

metab:

- name
- 'metab of ' + inform
- inform
- freund
- koc/1.724

substance_Macro:

- inform
- Koc
- halflife
- tref
- vap
- VpTemp
- pf
- expb
- tresp
- freund
- diffusion
- fstar
- convert

- inform
- Koc
- halflife
- tref
- vap
- VpTemp
- pf
- expb
- tresp
- freund
- diffusion * 86400
- fstar
- convert

** first metaboliet of parent:*

substances: (of parent)

- MetSubCode1

substances_PRZM: (of parent)

- icombo3

- name

- 2

** second metaboliet of parent:*

substances: (of parent)

- MetSubCode2

substances_PRZM: (of parent)

- icombo3

- name

- 3

3.5.3 Export substances to MACRO

At the end of SWASH or when the user starts the MACRO shell, all substances are exported to the MACRO database. First all substances in the MACRO *compound* and *metab* table are removed. The information MACRO needs of a compound is stored in the SWASH table *substance_Macro*. So the contents of this SWASH table is copied into the MACRO table *compound* or *metab*. All substances which are marked as parent go to table *compound*. Substances not marked as parent or substances used as metabolite are exported to table *metab*. In the MACRO table *metab* the field *inform* refers to the parent substance.

MACRO

If Parent then:

Compound:

- name
- Koc
- halflife
- tref
- vap
- VpTemp
- pf
- expb
- tresp
- freund
- diffusion
- fstar
- fext
- candeg

- inform
- FOCUStest

If Parent Compound has metabolites then:

** first metabolite*

Metab:

- name
- inform

** second metabolite*

Metab:

- name
- inform

If not Parent:

Metab:

- name
- Koc

SWASH

substance_Macro:

- substanceCode
- Koc
- halflife
- tref
- vap
- VpTemp
- pf
- expb
- tresp
- freund
- diffusion / 86400
- fstar
- fext / 1000
- candeg

substances:

- name
- Locked

substances:

- MetSubCode1
- SubstanceCode

substances:

- MetSubCode2
- SubstanceCode

substance_Macro:

- substanceCode
- Koc

- | | |
|-------------|---------------------|
| - halflife | - halflife |
| - tref | - tref |
| - vap | - vap |
| - VpTemp | - VpTemp |
| - pf | - pf |
| - expb | - expb |
| - tresp | - tresp |
| - freund | - freund |
| - diffusion | - diffusion / 86400 |
| - fstar | - fstar |
| - fconvert | - fconvert |

3.5.4 Import substances from PRZM

PRZM stores its substance data in a data file chmdat.dat. The record structure contains three parts (see Appendix 3). One for the parent chemical and two parts for the metabolites. In the SWASH database the field IsParent (table *substances*) indicates whether a substance is a parent (true) or a metabolite (false).

Reading one record from the data file means importing 3 substances in SWASH. Index i indicates parent (1), first metabolite (2) or second metabolite(3).

<u>SWASH</u>	<u>defaults</u>	<u>PRZM</u>
substances:		
<i>for new substances:</i>		
- SubstanceCode		- pstname[i]
- IsParent		- true (parent) or false (metabolite)
- Name		- pstname[i]
- Locked	false	
<i>if not locked:</i>		
- name		- pstname[i]
- KocSol		- kdsp[i]
- SlbWatRef		- solub[i]
- MolMass		- mwght[i]
- MolEntVap		- enpy[i]*1000/4.18
- CofDifAirRef		- dair[i]/10000
<i>if parent:</i>		
- MetSubCode1		- pstname[2]
- MetSubCode2		- pstname[3]
substance_PRZM:		
- SubstanceCode		- pstname[i]
- pstnam		- pstname[i]
- icheck1		- icheck1
- icheck2		- icheck2
- icheck3		- icheck3

if i = 1 then	
- icombo3	- icombo3
else	
- icombo3	- 0
- icheck5	- icheck5
- iqfac	- iqfac
- kdtyp	- kdtyp [i]
- apptyp	- apptyp [i]
- apparel	- apparel [i]
- dknum	- dknum [i]
- napp	- napp [i]
- kdsp	- kdsp [i]
- drate1a	- drate1a [i]
- drate1c	- drate1c [i]
- drate2a	- drate2a [i]
- fextrc	- fextrc [i]/100
- q10fac	- q10fac [i]
- qbase	- qbase [i]
- prtrn12	- prtrn12
- prtrn13	- prtrn13
- prtrn23	- prtrn23
- dtr121a	- dtr121a
- dtr121b	- dtr121b
- dtr121c	- dtr121c
- dtr122a	- dtr122a
- dtr131a	- dtr131a
- dtr131b	- dtr131b
- dtr131c	- dtr131c
- dtr132a	- dtr132a
- dtr231a	- dtr231a
- dtr231b	- dtr231b
- dtr231c	- dtr231c
- dtr232a	- dtr232a
- mseff	- mseff [i]
- mslab	- mslab [i]
- solub	- solub [i]
- mwght	- mwght [i]
- iset1	- iset1
- iset2	- iset2
- iset3	- iset3

substance_Macro:

- candeg	- pldkrt[i]
- feurnd	- frndcf [i]
- vap	- vp [i]
- fstar	- uptkf [i]

3.5.5 Export substances to PRZM

SWASH gets all parents from the *substance* table, if necessary adds the information of the metabolites and writes this to the PRZM datafile *chmdat.dat*. The number of written records to the datafile is written in the other datafile *chmnum.dat*.

3.5.6 Crop names

Every model should use these crop names. When SWASH creates a project (see Chapter 4) a subdirectory is created for each crop in a project using the name of the crop. As some characters cause problems these are replaced by underscore characters. The names in the second column are used as directory names.

MACRO doesn't know early or late applications. For MACRO this part of the crop name is omitted.

Name	Directory name
Appln, aerial	
Appln, hand (crop < 50 cm)	
Appln, hand (crop > 50 cm)	
Cereals, spring	Cereals_spring
Cereals, winter	Cereals_winter
Citrus	Citrus
Cotton	Cotton
Field beans	Field_beans
Grass/alfalfa	Grass_alfalfa
Hops	Hops
Legumes	Legumes
Maize	Maize
no drift (incorp or seed trtmt)	
Oil seed rape, spring	Oil_seed_rape_spring
Oil seed rape, winter	Oil_seed_rape_winter
Olives	Olives
Pome/stone fruit, early applns	Pome_stone_fruit_early_applns
Pome/stone fruit, late applns	Pome_stone_fruit_late_applns
Potatoes	Potatoes
Soybeans	Soybeans
Sugar beets	Sugar_beets
Sunflowers	Sunflowers
Tobacco	Tobacco
Vegetables, bulb	Vegetables_bulb
Vegetables, fruiting	Vegetables_fruiting
Vegetables, leafy	Vegetables_leafy
Vegetables, root	Vegetables_root

Vines, early applns	Vines_early_applns
Vines, late applns	Vines_late_applns

3.5.7 Scenarios

For the scenarios or locations the next coding should be used:

LocationCode	Weather station	
D1	Lanna (S)	DRAINAGE
D2	Brimstone (UK)	DRAINAGE
D3	Vredepeel (NL)	DRAINAGE
D4	Skousbo (DK)	DRAINAGE
D5	La Jailliere (F)	DRAINAGE
D6	Thiva (GR)	DRAINAGE
R1	Weiherbach (D)	RUNOFF
R2	Porto (P)	RUNOFF
R3	Bologna (I)	RUNOFF
R4	Roujan (F)	RUNOFF

4 Creating projects

In SWASH the user creates projects. Each project is characterised by one substance (table *projects*). Therefore it has a link to the *substances* table with all the information about the substance.

Each project has one or more runs (table *runs*). This means for one substance several runs can be defined. Each run is characterised by a location, crop and waterbody type and has a specified application scheme (table *applications*).

SWASH searches for every possible combination of location, crop and waterbody type. For each combination SWASH creates a run for the parent substance. If the parent substance has metabolites, a run is created for each metabolite.

Each run has a RunID which is unique for all models and has the format: *xxxxxw_pm*.

xxxxx: 5-digit number for maximally 99999 runs.
w: indicates waterbody type: d=Ditch, s=Stream, p=Pond
pm: pa=Parent substance, m1=first metabolite, m2=second metabolite

NB: if a parent substance has two parallel metabolites then for the second metabolite an extra run is created with a new number and an extra run for the parent substance. (This is needed to meet requirements of the MACRO model.)

Below two examples are presented, that illustrate how runid's are allocated to the various runs of the different models.

Example 1: fictitious crop in D2 and R1 for a parent and two parallel metabolites, runid starting at 30

Scenario	Waterbody	Parent/meta	Runid SWASH	Runid MACRO or PRZM
D2	Ditch	Parent	00030d_pa	Macro00030_p.m2t
D2	Ditch	Meta1	00030d_m1	Macro00030_m.m2t
D2	Ditch	Parent	00031d_pa	Macro00031_p.m2t
D2	Ditch	Meta2	00031d_m1	Macro00031_m.m2t
D2	Stream	Parent	00030s_pa	Macro00030_p.m2t
D2	Stream	Meta1	00030s_m1	Macro00030_m.m2t
D2	Stream	Parent	00031s_pa	Macro00031_p.m2t
D2	Stream	Meta2	00031s_m1	Macro00031_m.m2t
				Please note that macro00031_p.m2t exists, but is identical to macro00030_p.m2t
R1	Pond	Parent	00032p_pa	00032_C1.p2t
R1	Pond	Meta1	00032p_m1	00032_C2.p2t
R1	Pond	Meta2	00032p_m2	00032_C3.p2t
R1	Stream	Parent	00032s_pa	00032_C1.p2t
R1	Stream	Meta1	00032s_m1	00032_C2.p2t
R1	stream	Meta2	00032s_m2	00032_C3.p2t
				Please note that only one PRZM run is needed

Example 2: fictitious crop at D4 and R1 for a parent and two (consecutive) metabolites, one being formed from the first metabolite, runid starting at 40

Scenario	waterbody	Parent/metabolite	Runid SWASH=TOXSWA	Runid MACRO or PRZM
D4	Pond	Parent	00040p_pa	Macro00040_p.m2t
D4	Pond	Meta1	00040p_m1	Macro00040_m.m2t
D4	Stream	Parent	00040s_pa	Macro00040_p.m2t
D4	Stream	Meta1	00040s_m1	Macro00040_m.m2t
				Please note that MACRO cannot handle meta2
R1	Pond	Parent	00041p_pa	00041_C1.p2t
R1	Pond	Meta1	00041p_m1	00041_C2.p2t
R1	Pond	Meta2	00041p_m2	00041_C3.p2t
R1	Stream	Parent	00041s_pa	00041_C1.p2t
R1	Stream	Meta1	00041s_m1	00041_C2.p2t
R1	stream	Meta2	00041s_m2	00041_C3.p2t
				Only one PRZM run needed

One of the main functions of SWASH is the preparation of input for the MACRO, PRZM and TOXSWA models. This consist of three parts: Creating a project report, files required to run PRZM and preparing the MACRO database. SWASH also updates some tables in the SWASH database to prepare for TOXSWA.

When the user creates a project he has to enter a path for the project. Default path is C:\SWASHProjects\. The directory is always the project name. At this directory all input and output will be written. The next structure is created in case of the default path name and a project called 'test' with scenarios for 2 crops:
(Files in *italic* are created by SWASH, rest are model output files)

```
C:\SWASHProjects\test
    \MACRO                test_report.txt
        \crop1            *.M2T
        \crop2            *.M2T
    \PRZM\
        \crop1            *.P2T, *.zip, *.pzm
        \crop2            *.P2T, *.zip, *.pzm
    \TOXSWA                *.txw
```

SWASH maintains for PRZM a file with a listing of all created projects. This file, przm.prj is located at the main directory of the PRZM application. It has the next record structure:

```
1-20:      Projectname      // EPPOA
21-100:    Projectpath      // C:\SWASHprojects\EPPOA
101-117:   CreationDate     // 26-Nov-2001-09:49
```

4.1 Project Report

SWASH creates a report file (<projectname>_report.txt) with a listing of all created runs and its application pattern. The report also shows the Mean Deposition and Mass Loading from the drift calculation. This report is a guideline for the user, it gives an overview of all runs to be performed with the various models.

4.2 Files for PRZM

PRZM has only runs to do for the runoff scenarios. For each crop in the project a pzm-file is created. It is located at the PRZM\crop subdirectory. This file is read by PRZM and contains all information it needs to do a run. The file is structured like a windows ini-file and looks like this:

```
[generalsettings]
ProjectName=Eppoa
SubstanceCode=EPPOA
Relationship=1           // one, two or no metabolites
CropCode=Legumes
R1=00005                // run ids
R2=00006
R3=00007
R4=00008

[Applications]         // Application pattern is identical for
all runs
AppMethod=ground spray
NumberOfApp=1
// Rate  CAM   Depi Foliar  Perc
1= 1.00  0    4.0  0      0.0

[R1]
FirstDayYrApp=91       // first possible day in year of
LastDayYrApp=121      // last possible day in year of
MinIntervalApps=1     // minimum interval in days between

[R2]
FirstDayYrApp=96
LastDayYrApp=126
MinIntervalApps=1

[R3]
FirstDayYrApp=97
LastDayYrApp=127
MinIntervalApps=1

[R4]
FirstDayYrApp=97
LastDayYrApp=127
MinIntervalApps=1
```

Corresponding application methods:

<u>PRZM</u>	<u>SWASH</u>
A	air appl.
AB	air blast
G	granular appl.
GS	ground spray
S	soil incorp.

For some application methods additional information is required in PRZM such as CAM values (Chemical Application Method) and Foliar.

<u>CAM</u>	<u>App. Method</u>	<u>Depth</u>	<u>Perc. top 2 cm</u>
1 = soil exponential	A,AB,GS		
2 = foliar linear	A,AB,GS		
3 = foliar exponential	A,AB,GS		
4 = uniform	G	x	
5 = furrow	G	x	
6 = surface	not in SWASH		
7 = T-band	G	x	x
8 = shank	not in SWASH		

Defaults values:

<u>App.method</u>	<u>Foliar</u>	<u>CAM</u>	<u>Depth</u>
A	yes	2	4
	no	1	4
AB	yes	2	4
	no	1	4
G	yes	4 [5,7]	10
	no	4 [5,7]	10
GS	yes	2	4
	no	1	4

4.3 Preparing MACRO database

Preparing the MACRO database means exporting the created runs in the project to the MACRO database. (See 3.5.1 Export runs to MACRO).

MACRO uses the same application methods as SWASH. However in the MACRO database it is stored in the table *run* as a number in the *app_method* field:

<u>SWASH</u>	<u>MACRO</u>
air appl.	0
air blast	1
granular appl.	2
ground spray	3
soil incorp.	4

4.4 Preparing TOXSWA database

TOXSWA uses the SWASH database. To prepare the database for TOXSWA some tables are updated.

- Table *ToxswaMap*
 - MapID: create new id
 - Name: projects.Name
 - Description: projects.Description
 - ModificationDate: Now
- Table *ToxswaMap*
 - MapID: create new id
 - ProjectID: projects.ProjectID
- Table *SimulationParameters*
 - RunID: Runs.RunID
 - StartDate: Default startdate simulation (see 4.4.1)
 - EndDate: Default enddate simulation (see 4.4.1)
 - OpLatEntryModel: 2 (PRZM/MACRO)
 - LatEntryFile: MACRO_M2T or PRZM_P2T filename
- Table *ApplicationSchemes*
 - ApplicationSchemeID 12345xy
12345 = first part of RunID
x-value: 1 = Ditch
2 = Pond
3 = Stream
y-value: 0 = parent
1 = first metabolite
2 = second metabolite
 - Name AppScheme_ + aRun.RunID
 - EndDistanceDrift 100 (if POND then 30)
 - EndDistanceLatEntry 100 (if POND then 30)
 - RatioUpstreamBound 0.2 (if STREAM)
- Table *ToxswaApplications*
 - ApplicationNr Applications.ApplicationNr
 - SchemeID ApplicationSchemes.SchemeID
 - Rate Applications. Rate
 - CAM Applications. CAM
 - Depi Applications. Depi
 - Perc Applications. Perc
 - Foliar Applications. Foliar
 - SprayDrift 1
 - PercOfRate Calculated SprayDrift by Calculator

4.4.1 Default Simulation dates

Scenario	StartDate	EndDate
D1	01-Jan-1982	30-Apr-1983
D2	01-Jan-1986	30-Apr-1987
D3	01-Jan-1992	30-Apr-1993
D4	01-Jan-1985	30-Apr-1986
D5	01-Jan-1978	30-Apr-1979
D6	01-Jan-1986	30-Apr-1987

Scenario	first day of application	StartDate	EndDate
R1	March - May	01-Mar-1984	28-Feb-1985
R1	June - Sept	01-Jun-1978	31-May-1979
R1	Oct - Feb	01-Oct-1978	30-Sep-1979
R2	March - May	01-Mar-1977	28-Feb-1978
R2	June - Sept	01-Jun-1989	31-May-1990
R2	Oct - Feb	01-Oct-1977	30-Sep-1978
R3	March - May	01-Mar-1980	28-Feb-1981
R3	June - Sept	01-Jun-1975	31-May-1976
R3	Oct - Feb	01-Oct-1980	30-Sep-1981
R4	March - May	01-Mar-1984	28-Feb-1985
R4	June - Sept	01-Jun-1985	31-May-1986
R4	Oct - Feb	01-Oct-1979	30-Sep-1980

5 Installation & Software Requirements

The installation procedure only includes the installation of SWASH. Versions of MACRO, PRZM or TOXSWA should be installed at subdirectories of SWASH. The FOCUS Version Control Workgroup takes care of version control of the various tools. The SWASH developer has made 'Installation and Communication requirements' protocols for the various tools, to which each model update should comply (Appendix 4, 5 and 6).

SWASH is default installed at the directory C:\SWASH. The user has the possibility to choose another drive. However versions of PRZM, MACRO and SWASH must be installed at a subdirectory of the chosen drive. (See Appendix 7 for details.)

At that drive the next structure is created:

```
C:\SWASH          SWASH-applicationfiles
  \DATA           SWASH_db.mdb
    \MAPS         map-files
  \MACRO          <MACRO-applicationfiles>
  \PRZM           <PRZM-applicationfiles, przm.prj>
    \MET
    \PROGS
    \T3G
    \WPIC         <chmdat.dat, chmnum.dat>
  \TOXSWA        <TOXSWA-applicationfiles>
    \Pictures     <*.jpg>
```

Files between <> are not installed during the SWASH installation. Installations of MACRO, PRZM or TOXSWA take care of that.

SWASH requires a PC with a Windows version 98 or higher with MSAccess 97 or higher. It needs 6.5 Mb for installation

SWASH has been developed with the Delphi Development Environment. Normally Delphi uses the BDE (Borland Database Engine) to communicate with databases. However Borland did not update the BDE with drivers for MS-Access 2000 databases. New PCs with Win2000 and Office2000 cannot read the SWASH and MACRO databases. Therefore SWASH uses ODBC instead of the BDE. In Delphi ADO-components are used instead of the BDE-components.

SWASH has been tested on Win2000, WinNT and WinXP. SWASH is likely to run on Win95 and Win 98 machines, however, this has not yet been tested.

Win2000 has been combined with MS Office Access97, and with MS office Access2000, without prior Access 97 installed.

WinNT has been tested with MS Office Access97.

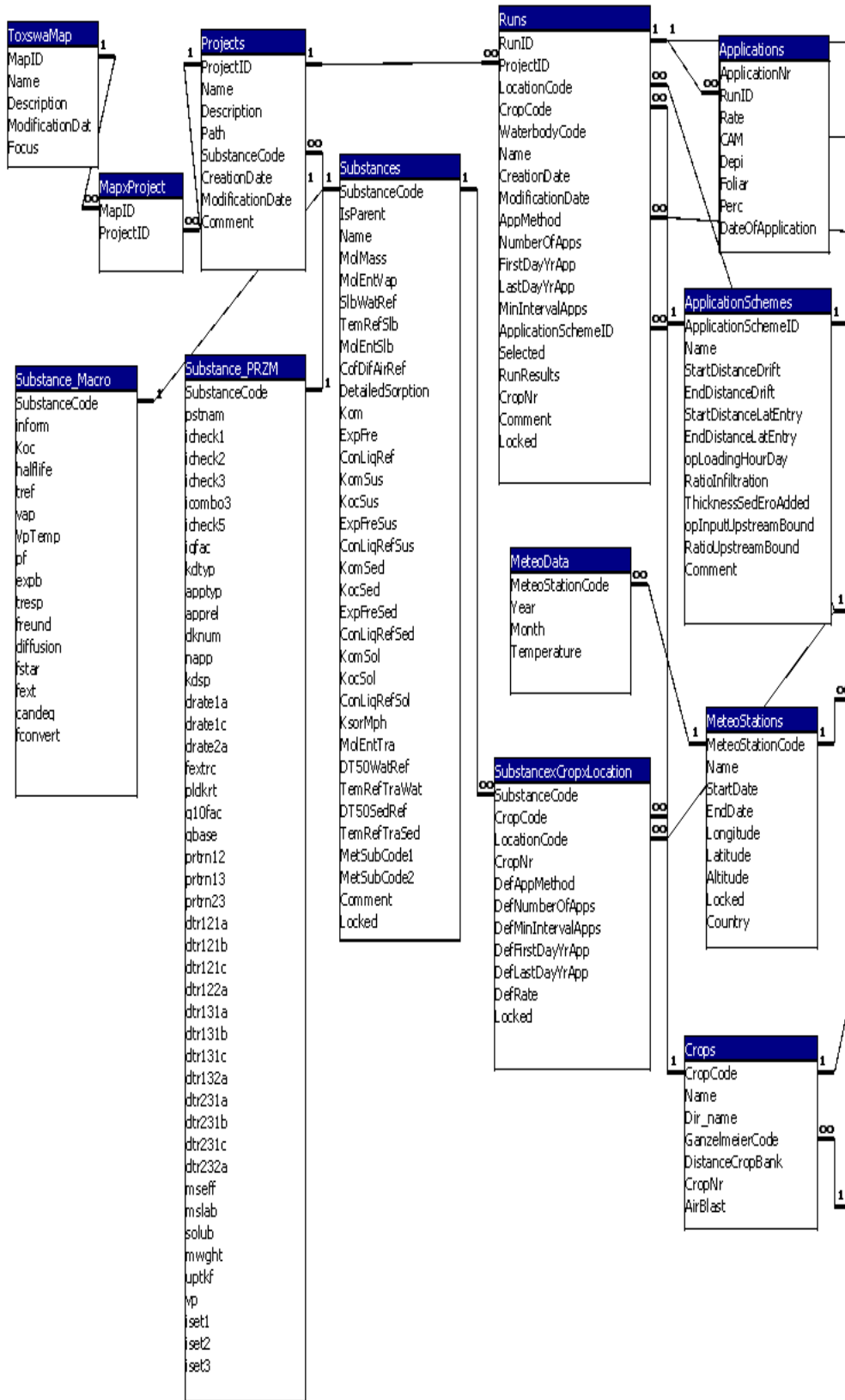
WinXp has been tested with MS Office AccessXP.

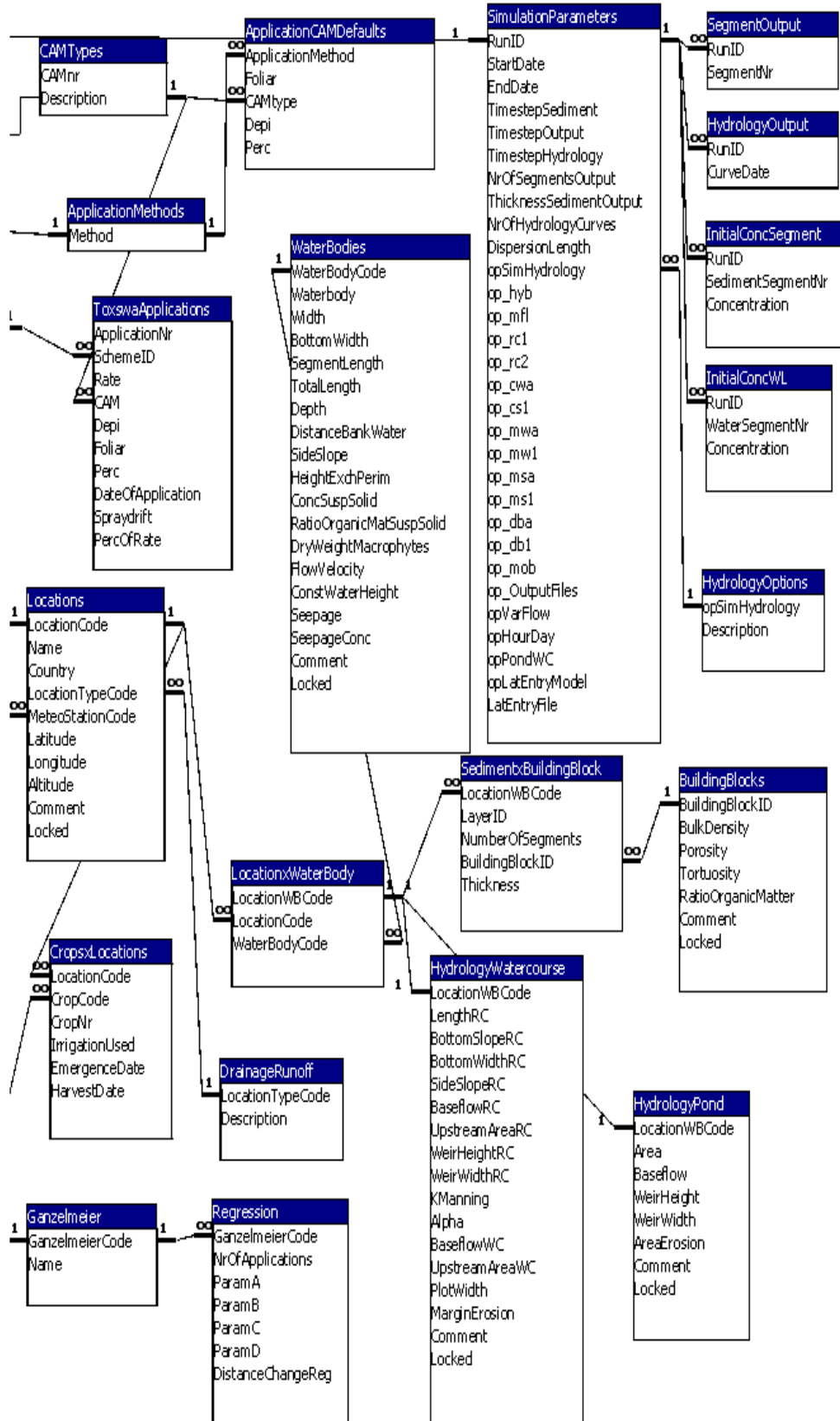
References

Berg, F. van den, P.I. Adriaanse and J.A. te Roller, 2002 Surface Water Scenarios Help (SWASH), version 1.9, User's Guide, version 1.2, Alterra-rapport 507, Wageningen, the Netherlands.

FOCUS, 2002 FOCUS Surface Water Scenarios in the EU Evaluation Process under 91/414/EEC. Report of the FOCUS Working Group on Surface Water Scenarios, EU Document Reference SANCO/4802/2002, rev.1.221 pp

Appendix 1 . SWASH/TOXSWA database relationships

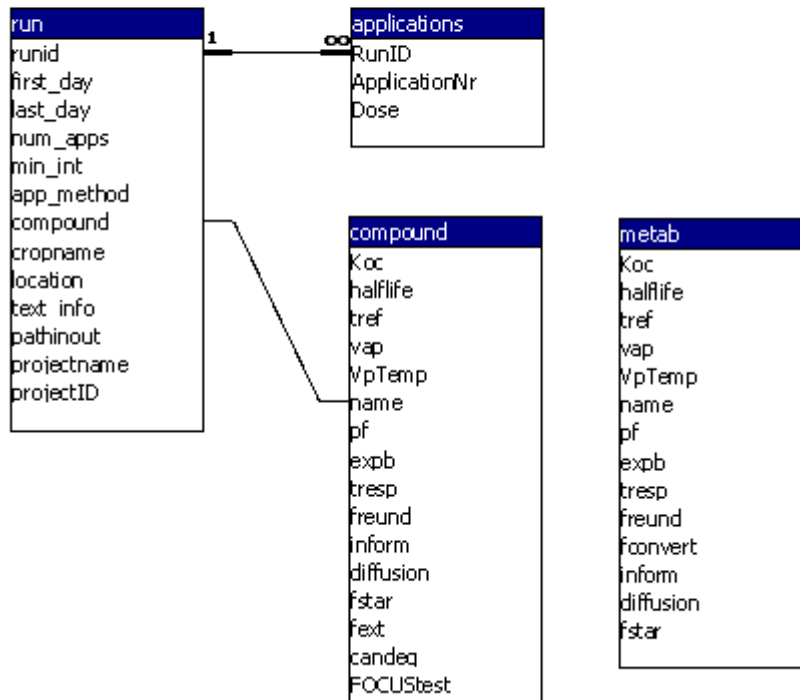




Appendix 2 . MACRO database relationships

Relationships for pest_focus

donderdag 26 september 2002



Appendix 3 . PRZM datafile structure CHMDAT.DAT

This part of a fortran subroutine shows the record structure of the data file chmdat.dat.

```
      SUBROUTINE GETCHM
      !
      ! Gets values of chemical from database and puts them into
      ! dialog fields.
      !
      200
      FORMAT(A20,A20,9(I1),I3,I2,e10.4,9(F7.2),A20,3(I1),I3,I2,e10.4,13(F7.2), &
      A20,3(I1),I3,I2,e10.4,17(F7.2),I1,6(F7.3),3(E10.4),6(F7.3),3(E10.4),4I1,&
      15I5,15F5.2,6F8.3)
      OPEN(21,FILE=DRVLTTR/'\SWASH\PRZM\WPIC\CHMDAT.DAT', &
      STATUS='UNKNOWN', &
      ACCESS='DIRECT', &
      FORM='FORMATTED',RECL=760)
      READ(21,200,REC=NOPT1) SUBCODE, &
      PSTNAM(1),ICHECK1,ICHECK2,ICHECK3,ICOMBO3, &
      ICHECK5,IQFAC,KDTYP(1),APPTYP(1),APPREL(1),DKNUM(1), &
      NAPP(1),KDSP(1),DRATE1A(1),FRNDCF(1),DRATE1C(1), &
      DRATE2A(1),FEXTRC(1),PLDKRT(1),PRTRN12,Q10FAC(1),QBASE(1), &
      PSTNAM(2),KDTYP(2),APPTYP(2),APPREL(2),DKNUM(2),NAPP(2), &
      KDSP(2),DRATE1A(2),FRNDCF(2),DRATE1C(2),DRATE2A(2), &
      DTR121A,DTR121B,DTR121C,DTR122A,FEXTRC(2),PLDKRT(2), &
      PRTRN13,Q10FAC(2),QBASE(2), &
      PSTNAM(3),KDTYP(3),APPTYP(3),APPREL(3),DKNUM(3),NAPP(3), &
      KDSP(3),DRATE1A(3),FRNDCF(3),DRATE1C(3),DRATE2A(3),DTR131A, &
      DTR131B,DTR131C,DTR132A,DTR231A,DTR231B,DTR231C,DTR232A, &
      FEXTRC(3),PLDKRT(3),PRTRN23,Q10FAC(3),QBASE(3),IQFAC, &
      (MSEFF(K),K=1,3),(MSLAB(K),K=1,3),(SOLUB(K),K=1,3), &
      (MWGHT(K),K=1,3),(UPTKF(K),K=1,3),(VP(K),K=1,3),ISET1,ISET2,ISET3, &
      ICHECK6,((KDDAYS(K,I),I=1,5),K=1,3),((KDFAC(K,I),I=1,5),K=1,3), &
      (ENPY(K),K=1,3),(DAIR(K),K=1,3)
      CLOSE(21)
      IF(ICHECK3.EQ.0)IQFAC=0
      !
      RETURN
      END SUBROUTINE GETCHM
```

Variable Definitions (Note: (1)=chemical 1 (2)=chemical 2 (3)=chemical 3)

SUBCODE	Substance Code
PSTNAM(1)	Pesticide name of chemical 1
ICHECK1	Flag for bi-phase degradtion
ICHECK2	Flag for Foliar applications
ICHECK3	Flag for Freundlich isotherm (non-linear adsorption)
ICOMBO3	Parent/Metabolite relationship
ICHECK5	Flag for volatilization
IQFAC	Flag for soil temperature/moisture degradation correction
KDTYP(1)	Soil Partition type
APPTYP(1)	Application type
APPREL(1)	Application timing
DKNUM(1)	Second Phase 1/2-life beginning relative to 1st application
NAPP(1)	# of applications
KDSP(1)	Soil Partition value

DRATE1A(1) 1/2-life days phase 1
 FRNDCF(1) Freundlich coefficient
 DRATE1C(1) unused in INFOCUS PRZM
 DRATE2A(1) 1/2-life days phase 2
 FEXTRC(1) Foliar Extraction
 PLDKRT(1) Foliar Decay rate
 PRTRN12 % transfer of parent degradation on foliage
 Q10FAC(1) q10 factor
 QBASE(1) q10 base temperature
 PSTNAM(2) Pesticide name of chemical 2
 KDTYP(2) Soil Partition type
 APPTYP(2) Application type
 APPREL(2) Application timing
 DKNUM(2) Second Phase 1/2-life beginning relative to 1st application
 NAPP(2) # of applications
 KDSP(2) Soil Partition value
 DRATE1A(2) 1/2-life days phase 1
 FRNDCF(2) Freundlich coefficient
 DRATE1C(2) unused in INFOCUS PRZM
 DRATE2A(2) 1/2-life days phase 2
 DTR121A % transfer of parent degradation in soil phase 1
 DTR121B unused in INFOCUS PRZM
 DTR121C unused in INFOCUS PRZM
 DTR122A % transfer of parent degradation in soil phase 2
 FEXTRC(2) Foliar Extraction
 PLDKRT(2) Foliar Decay rate
 PRTRN13 % transfer of parent degradation on foliage
 Q10FAC(2) q10 factor
 QBASE(2) q10 base temperature
 PSTNAM(3) Pesticide name of chemical 3
 KDTYP(3) Soil Partition type
 APPTYP(3) Application type
 APPREL(3) Application timing
 DKNUM(3) Second Phase 1/2-life beginning relative to 1st application
 NAPP(3) # of applications
 KDSP(3) Soil Partition value
 DRATE1A(3) 1/2-life days phase 1
 FRNDCF(3) Freundlich coefficient
 DRATE1C(3) unused in INFOCUS PRZM
 DRATE2A(3) 1/2-life days phase 2
 DTR131A % transfer of parent degradation in soil phase 1 (1->3)
 DTR131B unused in INFOCUS PRZM
 DTR131C unused in INFOCUS PRZM
 DTR132A % transfer of parent degradation in soil phase 2 (1->3)
 DTR231A % transfer of parent degradation in soil phase 1 (2->3)
 DTR231B unused in INFOCUS PRZM
 DTR231C unused in INFOCUS PRZM
 DTR232A % transfer of parent degradation in soil phase 2 (2->3)
 FEXTRC(3) Foliar Extraction
 PLDKRT(3) Foliar Decay rate
 PRTRN23 % transfer of parent degradation on foliage
 Q10FAC(3) q10 factor
 QBASE(3) q10 base temperature
 IQFAC Flag for soil temperature/moisture degradation correction
 (MSEFF(K),K=1,3) Soil Moisture correction factor (exponent)
 (MSLAB(K),K=1,3) Soil Moisture correction factor (lab moisture)
 (SOLUB(K),K=1,3) Solubility
 (MWGHT(K),K=1,3) Molecular weight
 (UPTKF(K),K=1,3) Uptake Factor
 (VP(K),K=1,3) Vapor Pressure
 ISET1 Moisture factor relative to FC or % chemical 1
 ISET2 Moisture factor relative to FC or % chemical 2
 ISET3 Moisture factor relative to FC or % chemical 3

ICHECK6 Flag soil moisture correction
((KDDAYS(K,I),I=1,5),K=1,3) unused in INFOCUS PRZM
((KDFAC(K,I),I=1,5),K=1,3) unused in INFOCUS PRZM
(ENPY(K),K=1,3) enthalpy of vaporisation of pesticide for chem K
(DIAR(K),K=1,3) diffusion coeff of pesticide in air for chem K

Appendix 4. Protocol for installation and communication requirements of MACRO for SWASH

Whenever the MACRO Model Developer intends to release a new version of the FOCUS MACRO-SW he should take care that this new version fulfills the agreed installation procedure under the SWASH tool as well as the requirements for communication between FOCUS MACRO-SW and SWASH. The installation and communication requirements are specified below.

1. Installation

When SWASH is installed, the following directory structure is created by the installation software:

```
C:\SWASH                SWASH-application files
  \MACRO                MACRO-application files
  \PRZM                 PRZM-application files, przm.prj
    \MET
    \PROGS
    \T3G
    \WPIC
  \TOXSWA              TOXSWA-application files
  \DATA                SWASH_db.mdb
    \MAPS              map files
```

Instead of C: another drive can be selected, e.g. D: or E:.

The MACRO Model Developer ensures that the following conditions are fulfilled during installation of MACRO:

- The complete MACRO tool should be placed in the subdirectory \MACRO. The MACRO Model Developer is free to create new subdirectories in this directory.
- The database **pest_focus.mdb** and the executable **MACRO_Focus.exe** are placed at the directory \MACRO, and not in a subdirectory.

2. Output

SWASH needs a project path to be able to save the various output files for a specific modelling project. The default path is C:\SWASHProjects\, but the user is able to select any other path. The project name is always the name of the directory. The following structure is created for project output files:

```
C:\SWASHProjects\testproject\MACRO\
  crop1                *.M2T
  crop2                *.M2T
  \PRZM\
    crop1              *.P2T, *.zip,
                      *.pzm
    crop2              *.P2T, *.zip,
                      *.pzm
  \TOXSWA              *.txw
```

The MACRO Model Developer ensures that the following conditions are fulfilled following completion of MACRO modelling:

- The M2T outputfiles should be placed at the correct output directory. The name of this directory should match the field **pathinout** from the table **run** in the database **pest_focus.mdb**. For each crop an output directory is created. Also the .bin, .log and .sum output files should be located in this same output directory.
- The M2T output files are named macro12345_p.M2T in case of a parent compound and macro12345_m.M2T in case of a metabolite. (Notice that MACRO can handle only one metabolite at a time, and so, in case of multiple metabolites originating from one parent, SWASH creates a second run with a next runid for MACRO.) The number 12345 corresponds to the communal, SWASH runid, which generally differs from the MACRO runid, mentioned in the names of the .bin, .log and .sum output files of MACRO.

3. Communication

SWASH updates the MACRO database **pest_focus.mdb**. Created substances in SWASH are exported to the tables **compound** and **metab**. Created runs in SWASH are exported to the tables **applications** and **run**.

The MACRO Model developer ensures that the following conditions are fulfilled:

- The structure and field names of the tables **compound**, **metab**, **applications** and **run** is not changed.
- The agreed names for crops and locations are used in the tables, i.e.

Crops:

Cereals, spring
Cereals, winter
Citrus
Cotton
Field beans
Grass/alfalfa
Hops
Legumes
Maize
Oil seed rape, spring
Oil seed rape, winter
Olives
Pome/stone fruit, early applns
Pome/stone fruit, late applns
Potatoes
Soybeans
Sugar beets
Sunflowers
Tobacco

Vegetables, bulb
Vegetables, fruiting
Vegetables, leafy
Vegetables, root
Vines, early applns
Vines, late applns

Locations: D1, D2, D3, D4, D5 and D6

More details have been described in:

Roller, J.A. te, F. van den Berg, P.I. Adriaanse, 2002. Surface Water Scenarios Help (SWASH), version 1.9. Technical report version 1.2, Alterra-rapport 508, Wageningen, the Netherlands.

4. Test project

(to go through by the MACRO Developer, before sending the new FOCUS MACRO_SW version to the FOCUS Version Control Working Group)

- Replace the old MACRO version with the new one.
- Start SWASH.
- Check the new MACRO version numbers from the SWASH tab sheet **information** option **versions**.
- Create a new substance in SWASH.
- Create a project in SWASH using the new substance.
- Create a project in SWASH using a FOCUS substance.
- Start the MACRO shell from SWASH.
- Run MACRO using the new substance and runs created in SWASH.
- Run MACRO using the FOCUS substance and runs created in SWASH.
- Check if the output files are generated at the correct directory.
- Exit MACRO and SWASH.

Appendix 5. Protocol for installation and communication requirements of PRZM for SWASH

Whenever the PRZM Model Developers intends to release a new version of the FOCUS_PRZM_SW they should take care that this new version fulfills the agreed installation procedure under the SWASH tool as well as the requirements for communication between FOCUS_PRZM-SW and SWASH. The installation and communication requirements are specified below.

1. Installation

When SWASH is installed the following directory structure is created by the installation software:

```
C:\SWASH                SWASH-application files
  \MACRO                MACRO-application files
  \PRZM                 PRZM-application files, przm.prj
    \MET
    \PROGS
    \T3G
    \WPIC
  \TOXSWA              TOXSWA-application files
  \DATA                SWASH_db.mdb
    \MAPS              map files
```

Instead of C: another drive can be selected, e.g. D: or E:.

The PRZM Model Developer ensures that the following conditions are fulfilled during installation of PRZM:

- The complete PRZM tool should be placed in the subdirectory \PRZM. The PRZM Model Developer is free to create new subdirectories in this directory.
- The **file versionnum.dat** and the executable **PFSW.exe** are placed at the directory \PRZM, and not in a subdirectory.
- The **files chmnum.dat** and **chmdat.dat** are placed at the subdirectory \PRZM\WPIC.

2. Output

SWASH needs a project path to be able to save the various output files for a specific modelling project. The default path is C:\SWASHProjects\, but the user is able to select any other path. The project name is always the name of the directory. The following structure is created for project output files:

```
C:\SWASHProjects\testproject\MACRO\
                                     crop1      *.M2T
                                     crop2      *.M2T
  \PRZM\
                                     crop1      *.P2T, *.zip,
                                     *.pzm
```

```

crop2          *.P2T, *.zip,
               *.pzm
\TOXSWA\      *.txw

```

The PRZM Model Developer ensures that the following conditions are fulfilled following completion of PRZM modelling:

- The P2T output files should be placed at the correct output directory. The name of this directory should match the **records 21-100** (projectpath) of the **przm.prj** file located at the main directory of the PRZM application. For each crop an output directory is created. All other output files should be also located in this same output directory. The **przm.pzm** file for the selected crop of this project is also located at this directory.
- The **P2T output files** are named 12345_C1.P2T, 12345_C2.P2T or 12345_C3.P2T. C1 refers to the parent compound and C2 and C3 to metabolites. The number 12345 corresponds to the communal, SWASH runid.

3. Communication

SWASH updates the PRZM data files **chmdat.dat** and **chmnum.dat**.

The PRZM Model developer ensures that the following conditions are fulfilled:

- The structure of the PRZM data files **chmdat.dat** and **chmnum.dat** is not changed.
- The agreed names for crops and locations are used in the tables, i.e.

Crops:

Cereals, spring
 Cereals, winter
 Citrus
 Cotton
 Field beans
 Grass/alfalfa
 Hops
 Legumes
 Maize
 Oil seed rape, spring
 Oil seed rape, winter
 Olives
 Pome/stone fruit, early applns
 Pome/stone fruit, late applns
 Potatoes
 Soybeans
 Sugar beets
 Sunflowers
 Tobacco
 Vegetables, bulb
 Vegetables, fruiting

Vegetables, leafy
Vegetables, root
Vines, early applns
Vines, late applns

Locations: R1, R2, R3 and R4

More details have been described in:

Roller, J.A. te, F. van den Berg, P.I. Adriaanse, 2002. Surface WAter Scenarios Help (SWASH), version 1.9. Technical report version 1.2, Alterra-rapport 508, Wageningen, the Netherlands.

4. Test project

(to go through by the PRZM Developers before sending the new FOCUS PRZM_SW to the FOCUS Version Control Working Group)

- Replace the old PRZM version with the new one.
- Start SWASH.
- Check the new PRZM version numbers from the SWASH tab sheet **information** option **versions**.
- Create a new substance in SWASH.
- Create a project in SWASH using the new substance.
- Create a project in SWASH using a FOCUS substance.
- Start the PRZM shell from SWASH.
- Run PRZM using the new substance and runs created in SWASH.
- Run PRZM using the FOCUS substance and runs created in SWASH.
- Check if the output files are generated at the correct directory.
- Exit PRZM and SWASH.

Appendix 6 . Protocol for installation and communication requirements of TOXSWA for SWASH

Whenever the TOXSWA Model Developers intends to release a new version of the FOCUS MACRO-SW they should take care that this new version fulfills the agreed installation procedure under the SWASH tool as well as the requirements for communication between FOCUS TOXSWA and SWASH. The installation and communication requirements are specified below.

1. Installation

When SWASH is installed, the following directory structure is created by the installation software:

```
C:\SWASH          SWASH-application files
  \MACRO          MACRO-application files
  \PRZM           PRZM-application files, przm.prj
    \MET
    \PROGS
    \T3G
    \WPIC
  \TOXSWA         TOXSWA-application files
  \DATA           SWASH_db.mdb
    \MAPS         map files
```

Instead of C: another drive can be selected, e.g. D: or E:.

The TOXSWA Model Developers ensure that the following conditions are fulfilled during installation of TOXSWA:

- The complete TOXSWA tool should be placed in the subdirectory \TOXSWA. The TOXSWA Model Developers are free to create new subdirectories in this directory.
- The executable **TOXSWA_FOCUS.exe** is placed at the directory \TOXSWA, and not in a subdirectory.
- The file **versionnum.dat** with the version numbers is updated and also placed at the directory \TOXSWA.

N.B. TOXSWA does **not** install a **swash_db.mdb**. This is done by SWASH !

2. Output

SWASH needs a project path to be able to save the various output files for a specific modelling project. The default path is C:\SWASHProjects\, but the user is able to select any other path. The project name is always the name of the directory. The following structure is created for project output files:

```

C:\SWASHProjects\testproject\MACRO\
                                crop1      *.M2T
                                crop2      *.M2T
                                \PRZM\
                                crop1      *.P2T, *.zip,
                                         *.pzm
                                crop2      *.P2T, *.zip,
                                         *.pzm
                                \TOXSWA    *.txw

```

The TOXSWA Model Developers ensure that the following conditions are fulfilled following completion of TOXSWA modelling:

- The M2T output files should be read from the correct MACRO crop directory.
- The P2T output files should be read from the correct PRZM crop directory.
- The txw-files and TOXSWA output files should be placed at the TOXSWA directory.

3. Communication

SWASH and TOXSWA make use of the same database. This implies that

The TOXSWA Model Developers ensure that the following conditions are fulfilled:

- The structure and field names of **all tables** of the **SWASH-db.mdb** are not changed.
- The agreed names for crops and locations are used in the tables, i.e.

Crops:

Cereals, spring
 Cereals, winter
 Citrus
 Cotton
 Field beans
 Grass/alfalfa
 Hops
 Legumes
 Maize
 Oil seed rape, spring
 Oil seed rape, winter
 Olives
 Pome/stone fruit, early applns
 Pome/stone fruit, late applns
 Potatoes
 Soybeans
 Sugar beets
 Sunflowers
 Tobacco
 Vegetables, bulb
 Vegetables, fruiting
 Vegetables, leafy

Vegetables, root
Vines, early applns
Vines, late applns

Locations: D1, D2, D3, D4, D5, D6, R1, R2, R3 and R4

More details have been described in:

Roller, J.A. te, F. van den Berg, P.I. Adriaanse, 2002. Surface WATER Scenarios Help (SWASH), version 1.9. Technical report version 1.2, Alterra-rapport 508, Wageningen, the Netherlands.

4. Test project

(to go through by the TOXSWA Developers, before sending the new FOCUS TOXSWA version to the FOCUS Version Control Working Group)

- Replace the old TOXSWA version with the new one.
- Start SWASH.
- Check the new TOXSWA version numbers from the SWASH tab sheet **information** option **versions**.
- Create a new substance in SWASH.
- Create a project containing D scenarios in SWASH using the new substance.
- Create a project containing R scenarios in SWASH using a FOCUS substance.
- Start the MACRO shell from SWASH
- Run MACRO using the new substance and runs created in SWASH
- Check if the output files are created at the correct directory
- Exit the MACRO shell and enter SWASH
- Start the PRZM shell from SWASH
- Run PRZM using the FOCUS substance and runs created in SWASH
- Check if the output files are created at the correct directory
- Exit the PRZM shell and enter SWASH
- Start the TOXSWA shell from SWASH.
- Run TOXSWA for a D scenario using the new substance and runs created in SWASH and check that the correct M2T file is read into TOXSWA.
- Run TOXSWA for a R scenario using the FOCUS substance and runs created in SWASH and check that the correct P2T file is read into TOXSWA.
- Check if the output files are generated at the correct directory.
- Exit TOXSWA and SWASH.

Appendix 7 . Read_me file for installation of the SWASH software package

SWASH Read_me_first file, date: 11-Oct-2002, version: 1

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This readme file contains information for

SWASH model=shell version 1.9
SWASH/TOXSWA database version 2.1 (11 October 2002)

Help

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If you suffer from installation problems or problems in the use of SWASH, send an e-mail to:

j.a.teroller@wisl.nl

Installation

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The complete installation of the SWASH software package includes five steps.

We can only guarantee a proper functioning of the entire package, if you install all applications on the default directory. The default directory for SWASH is C:\SWASH.

You may also choose another drive, for example D or F. In case you select another drive than C, the other applications should also be installed on that drive and as subdirectories of the SWASH directory. For example if you installed SWASH on

D:\SWASH the other applications should be installed at:

TOXSWA: D:\SWASH\TOXSWA
MACRO: D:\SWASH\MACRO
PRZM: D:\SWASH\PRZM

Step 1. Regional settings (for MACRO)

- Check the regional settings on your pc: they should be set to a default national setting, without making any changes, i.e. do not select 'Swedish', and then change the number format from the default decimal comma to the decimal point. (Select My computer, Control panel, Regional options, Numbers to check.)

Step 2. Installation of SWASH

- If necessary, uninstall previous versions of the SWASH
- Copy the SWASH.zip archive to your local machine
- Unzip SWASH.zip
- Run the Setup.exe program and follow on screen instructions

- SWASH can now be started from the Start menu

Step 3. Installation of TOXSWA

- If necessary, uninstall previous versions of the TOXSWA
- Copy the TOXSWA.zip archive to your local machine
- Unzip TOXSWA.zip
- Run the Setup.exe program and follow on screen instructions
- TOXSWA can now be started from the Start menu

Step 4. Installation of MACRO

- See read_me_MACRO.txt

Step 5. Installation of PRZM

- See read_me_PRZM.txt

Hard and software requirements

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Operating systems:

SWASH has been tested on Win2000, WinNT and WinXP.
SWASH is likely to run on Win95 and Win 98 machines,
however, this has not yet been tested.

(Win2000 has been combined with MS Office Access97,
and with MS office Access2000, without prior Access 97 installed.
WinNT has been tested with MS Office Access97.
WinXp has been tested with MS Office AccessXP.)

Remark:

On some versions of WinNT problems can occur with
the ODBC-drivers. In that case try to run MDAC.
MDAC (Microsoft Data Access Components) is a tool
from Microsoft and you can download it for free from
the Microsoft internet site (www.microsoft.com).

Access rights:

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

Preinstalled software:

Windows version 98 or higher
MSAccess 97 or higher

Hard disk memory:

SWASH requires 6.5 Mb for installation.
TOXSWA requires 3.5 Mb for installation.

Display:

Monitor with at least 800x600, at 256 colors.

Processor:

The faster the better.

Literature:

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Roller, J.A. te, F. van den Berg, P.I. Adriaanse, 2002. SURface WATER Scenarios Help (SWASH), version 1.9. Technical report version 1.2, Alterra-rapport 508, Wageningen, the Netherlands.

Berg, F. van den, P.I. Adriaanse, J.A. te Roller, 2002. Surface WATER Scenarios Help (SWASH), version 1.9. User's Guide version 1.2, Alterra-rapport 507, Wageningen, the Netherlands.

Known bugs:

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