



Wettelijke Onderzoekstaken Natuur & Milieu

FOCUS_TOXSWA manual 4.4.2

User's Guide version 4

| WOt-technical report 14

W.H.J. Beltman, M.M.S. ter Horst, P.I. Adriaanse, A. de Jong & J. Deneer



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FOCUS_TOXSWA manual 4.4.2

This WOt-technical report was produced in accordance with the Quality Manual of the Statutory Research Tasks Unit for Nature & the Environment.

The contents of the report was reviewed by the Task force on Agriculture of the Netherlands Release and Transfer Register.

The 'WOt-technical reports' series presents the findings of research projects implemented for the Statutory Research Tasks Unit for Nature & the Environment by various centres of expertise. WOt-technical Report 14 presents the findings of a research project commissioned and funded by the Dutch Ministry of Economic Affairs (EZ).

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Statutory Research Tasks Unit for Nature & the Environment (WOT Natuur & Milieu)

Wageningen, October 2014

WOT-technical report 14

ISSN 2352-2739

Abstract

W.H.J. Beltman, M.M.S. ter Horst, P.I. Adriaanse, A. de Jong & J. Deneer (2014). *FOCUS_TOXSWA manual 4.4.2; User's Guide version 4*. Statutory Research Tasks Unit for Nature & the Environment (WOT Natuur & Milieu) , WOt-technical report 14. 130 p.; 64 fig.; 7 tab.; 19 ref. 7 Annexes.

The FOCUS_TOXSWA model calculates exposure concentrations of pesticides and their metabolites in watercourses and ponds. These concentrations are used in the pesticide registration procedure at EU level. The model concepts of TOXSWA are described briefly. The input files, output files, and the use of the graphical user interface to access the input and output are described. Input data are stored in a database. Pesticide entries resulting from drainage or runoff/erosion are accessed from separate files generated by FOCUS_MACRO and FOCUS_PRZM. Substance properties are accessed from the SPIN tool/database. Instructions for simulating a water-sediment study and a multi-year run are given.

Keywords: exposure concentration, FOCUS, metabolites, pesticides, sediment, surface water, TOXSWA

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The WOt-technical reports series is published by the Statutory Research Tasks Unit for Nature & the Environment (WOT Natuur & Milieu), part of Wageningen UR. This document is available from the secretary's office, and can be downloaded from www.wageningenUR.nl/wotnatuurenmilieu

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Preface

This manual replaces the manual which was provided with FOCUS_TOXSWA 2.2.1, and which was still suitable for FOCUS_TOXSWA 3.3.1. A complete redesign of the TOXSWA kernel, the Graphical User Interface and the database also required a new manual, describing the software and its use adequately. The result is the current manual for use of FOCUS_TOXSWA 4.4.2. The authors hope it will fulfil its aim, assisting first-time users in their first endeavours, and serving as a reference for more advanced users.

Wim Beltman

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Summary

The TOXSWA (TOXic substances in Surface WAters) model has been developed to calculate exposure concentrations for use in the ecotoxicological risk assessment of pesticides for the aquatic ecosystem. FOCUS_TOXSWA is used in the EU registration procedure. The TOXSWA model together with its Graphical User Interface (GUI) and database form the FOCUS_TOXSWA tool.

TOXSWA simulates the behaviour of pesticides and their metabolites in a water body at the edge-of-field scale, i.e. a ditch, pond or stream adjacent to a single, treated field. It calculates pesticide concentrations, Predicted Environmental Concentrations (PECs) and Time Weighted Average Exposure Concentrations (TWAECs), in both the water layer and the sediment. FOCUS_TOXSWA simulates a transient hydrology and can handle water fluxes and pesticide fluxes resulting from drainage, surface runoff (incl. erosion), as well as instantaneous pesticide entries via spray drift deposition. In order to simulate the flow dynamics in an edge-of-field water body in a realistic way, the field-scale system is characterized as the downstream part of a small catchment basin.

In TOXSWA four processes are considered: (i) transport, (ii) transformation, (iii) sorption and (iv) volatilisation. In the water layer pesticides are transported by advection and dispersion, while in the sediment diffusion is included as well. Sorption to suspended solids and to sediment is described by the Freundlich equation. Sorption to macrophytes is described by a linear sorption isotherm. Pesticides are transported across the water-sediment interface by advection (upward or downward seepage) and by diffusion. In the FOCUS surface water scenarios, transport across the water-sediment interface takes place by diffusion only. The water body system in TOXSWA is described using a water balance that accounts for all incoming and outgoing water fluxes. The variation of the water level in time is calculated in two different ways, for ponds and for watercourses (ditches and streams).

This report presents the FOCUS_TOXSWA 4.4.2 model. The most important new features of the FOCUS_TOXSWA model compared to the three previous FOCUS_TOXSWA versions 1.1.1, 2.2.1 and 3.3.1 are:

- metabolite formation in the water layer and in the sediment of the water body is considered,
- formation of primary metabolites in the water layer of the upstream catchment of FOCUS streams is included,
- simulation of multi-year runs,
- the substances sections of the GUI and of the database have been moved to a separate tool, called SPIN, and
- complete redesign of TOXSWA kernel, Graphical User Interface and database was accomplished.

FOCUS_TOXSWA is closely linked with the FOCUS_SWASH tool. SWASH has been developed to prepare all run inputs needed by the different FOCUS surface water tools for running FOCUS surface water scenarios.

The user can access the FOCUS_TOXSWA system through the Graphical User Interface (GUI). The GUI is linked with a relational database (SWASH/TOXSWA database) for easy data access. The GUI generates the input files for the TOXSWA model and calls the model. Summary of input and output can be viewed from within the TOXSWA GUI. More comprehensive outputs can be viewed using graphs that are prepared by the GUI. A user's guide for the command line version of FOCUS_TOXSWA has been included as well.

Setting up the simulations of a water-sediment study and of a multi-year run is demonstrated in a separate chapter.

Samenvatting

Het model TOXSWA (TOXic substances in Surface Waters) is ontwikkeld om blootstellingsconcentraties van gewasbeschermingsmiddelen te berekenen voor de ecotoxicologische risicobeoordeling van gewasbeschermingsmiddelen in aquatische ecosystemen. FOCUS_TOXSWA wordt gebruikt bij de EU-toelatingsprocedure. Het TOXSWA-model plus de bijbehorende Graphical User Interface (GUI) en database vormen samen het FOCUS_TOXSWA-instrument.

Met TOXSWA wordt het gedrag van gewasbeschermingsmiddelen en hun metabolieten gesimuleerd in een naast een met gewasbeschermingsmiddel behandeld landbouwperceel gelegen sloot, plas of klein riviertje. Piekconcentraties (Predicted Environmental Concentrations, PEC's) en concentraties voor chronische blootstelling (Time Weighted Average Exposure Concentrations, TWAEC's) worden berekend voor zowel de waterlaag als het sediment. FOCUS_TOXSWA simuleert een variabele hydrologie. Zowel water- als gewasbeschermingsmiddelfluxen die voortvloeien uit drainage, oppervlakkige afvoer (inclusief erosie) alswel directe belasting met gewasbeschermingsmiddelen door drift bij bespuitingen worden gesimuleerd. Om de stromingsdynamiek in een waterloop naast een landbouwperceel realistisch te simuleren, wordt de waterloop op veldschaal beschouwd als het benedenstroomse deel van een klein stroomgebied.

In TOXSWA worden vier processen gesimuleerd: (i) transport, (ii) omzetting, (iii) sorptie en (iv) vervluchtiging. In de waterlaag worden gewasbeschermingsmiddelen getransporteerd via advectie en dispersie, terwijl in het sediment diffusie ook een rol speelt. Sorptie aan zwevende stof en aan het sediment wordt beschreven met de Freundlich-vergelijking. Sorptie aan macrofyten wordt beschreven met een lineaire sorptie-isotherm. Het transport van gewasbeschermingsmiddelen door het grensvlak tussen waterlaag en sediment vindt plaats via advectie (opwaartse of neerwaartse kwel) en via diffusie. In de FOCUS-scenario's voor oppervlaktewater vindt het transport door het grensvlak water - sediment alleen plaats via diffusie. In TOXSWA wordt het te bestuderen systeem beschreven aan de hand van een waterbalans waarin opgenomen alle inkomende en uitgaande waterfluxen. De variatie in het waterpeil in de tijd wordt op twee verschillende manieren berekend, voor plassen en voor waterlopen (sloten en kleine riviertjes).

In dit rapport wordt FOCUS_TOXSWA versie 4.4.2 gepresenteerd. De voornaamste nieuwe eigenschappen van deze versie van FOCUS_TOXSWA ten opzichte van de drie eerdere versies (1.1.1, 2.2.1 en 3.3.1) zijn:

- de vorming van metabolieten in de waterlaag en in het sediment wordt ook gesimuleerd,
- de vorming van primaire metabolieten in de waterlaag van het bovenstroomse deel van het stroomgebied van FOCUS-kleine riviertjes wordt ook meegenomen,
- ook meerjarige simulaties zijn mogelijk,
- de delen van de GUI en de database die betrekking hebben op stoffen zijn ondergebracht in een apart instrument, SPIN geheten, en
- rekenhart, GUI en database van TOXSWA zijn geheel vernieuwd.

FOCUS_TOXSWA is nauw verbonden met het instrument FOCUS_SWASH. FOCUS_SWASH levert alle invoer voor de simulaties die door de verschillende FOCUS-modellen worden gedaan om de FOCUS-scenario's voor oppervlaktewater door te rekenen.

Gebruikers kunnen het FOCUS_TOXSWA-instrument benaderen via de Graphical User Interface (GUI). Deze GUI is verbonden met een relationele database (SWASH/TOXSWA database), waardoor gemakkelijk toegang kan worden verkregen tot de gegevens. De GUI genereert de invoerbestanden voor het model TOXSWA en start de simulaties met het model. Binnen de TOXSWA-GUI kan een samenvatting van de in- en uitvoer worden bekeken. Een meer uitgebreid overzicht van de uitvoergegevens kan worden bekeken via de grafieken die worden aangemaakt door de GUI. Er is een gebruikershandleiding beschikbaar voor de command line versie van FOCUS_TOXSWA.

In een afzonderlijk hoofdstuk (Hoofdstuk 5) wordt toegelicht hoe de simulaties voor een water - sedimentstudie en voor een meerjarige simulatie worden opgezet.

1 Introduction

1.1 General

This document is a guide to the use of TOXSWA (TOXic substances in Surface Waters), a simulation model developed to assess pesticide exposure concentrations (PECs) in water and in sediment, for use in the EU registration procedure. The TOXSWA model together with its Graphical User Interface (GUI) and database form the FOCUS_TOXSWA tool.

TOXSWA simulates the behaviour of pesticides in a water body at the edge-of-field scale, i.e. a ditch, pond or stream adjacent to a single, treated field. It calculates concentrations of pesticides and their metabolites in both the water layer and in the sediment. FOCUS_TOXSWA simulates a transient hydrology and water fluxes and pesticide fluxes resulting from drainage, surface runoff (incl. erosion), as well as instantaneous pesticide entries via spray drift deposition. In order to simulate the flow dynamics in an edge-of-field water body in a realistic way, the field-scale system is characterized as the downstream part of a small catchment basin.

The FOCUS_TOXSWA tool is closely linked to the FOCUS_SWASH tool (Fait *et al.*, 2013). SWASH prepares all inputs for scenarios, applications and substances (via SPIN, see below) needed by the different FOCUS surface water tools to run the FOCUS surface water scenarios. It sets up the standard Step 3 exposure calculations in which the FOCUS Drift Calculator, the FOCUS_MACRO tool for drainage entries, and the FOCUS_PRZM_SW tool for runoff/erosion entries have been coupled to the FOCUS_TOXSWA tool for fate in surface waters.

FOCUS_SWASH and FOCUS_TOXSWA both are linked to the SPIN tool (van Kraalingen *et al.*, 2013). SPIN used via SWASH prepares all substance inputs for all FOCUS surface water tools for Step 3 runs. Using SPIN through TOXSWA enables showing the substance inputs used, and the creation and/or editing of substances for Step 4 runs.

This user guide concerns the FOCUS_TOXSWA version 4.4.2, consisting of:

TOXSWA model	FOCUS version 4 (= 3.3.2.F4, March 2014)
TOXSWA shell	FOCUS version 4 (= 3.0.3 April 2014)
SWASH/TOXSWA database	FOCUS version 2 (= June 2013)

FOCUS_TOXSWA version 4.4.2 is linked to the FOCUS-SWASH version 4.2, consisting of:

SWASH model = shell	FOCUS version 4 (= 4.01, June 2013)
SWASH/TOXSWA database	FOCUS version 2 (= June 2013)

FOCUS_TOXSWA version 4.4.2 and FOCUS-SWASH version 4.2 are linked to SPIN consisting of:

SPIN model = shell	SPIN version 1 (= 1.1.1, March 2014)
SPIN database	SPIN version 1 (= 54, June 2013)

FOCUS_TOXSWA v.4.4.2 reads the output files *.m2t created by MACRO or *.p2t created by PRZM, which have been prepared with the aid of the SWASH and the MACRO or PRZM tool, respectively. The versions of MACRO and PRZM are stated in SWASH (tab: Information, button: Versions). The FOCUS Version Control Working Group is responsible for version control and distribution of all FOCUS tools.

1.2 Main improvements in FOCUS_TOXSWA 4.4.2

The main improvements in FOCUS_TOXSWA are:

Inclusion of simulation of the formation of metabolites in water and sediment and their behaviour (see Adriaanse *et al.*, 2014). The metabolite scheme supported by TOXSWA is flexible and can consist of metabolites formed in parallel or formed in sequence or by a combination of both. The theoretical background of metabolite formation has been described by Adriaanse *et al.* (2014). The formation and fate of metabolites in water and in sediment as well as the fate of parents and metabolites entered by drainage or by runoff (and erosion) can be handled in a single run. The GUI supports the new metabolite options. The database has changed compared to FOCUS_TOXSWA_3.3.1, because of the development of the SPIN application and the option to define metabolite schemes for the water layer and the sediment.

FOCUS stream scenarios include an upstream catchment of which 20% is treated with pesticide. The upstream catchment is not simulated. To take into account the formation of metabolite in the upstream catchment, a correction factor for metabolite formation in the water layer of the upstream catchment for mass originating from spray drift deposition and from lateral runoff or drainage entries is included. The procedure to calculate the correction factor is given by Adriaanse *et al.*, (2014). This correction factor has a default value of 1, representing worst case situations.

Simulation of pesticide water and sediment concentrations over several years (e.g. 20 years), due to pesticide drift and the entry of pesticides via runoff as well as drainage can be simulated in so-called multi-year runs. For the latter two entry routes, m2t/p2t files are needed covering the entire simulation period. Global maximum concentrations are reported for each simulated calendar year in the summary file.

The code of the simulation kernel FOCUS_TOXSWA 3.3.1 has been fully revised. The kernel of FOCUS_TOXSWA 4.4.2 is now organized in a modular way which facilitates easy model development and simplifies future updates. Consequently, the structure of the input and output files was changed.

FOCUS_TOXSWA 4.4.2 uses the application SPIN (Substance Plug IN) to create and/or edit a) substances and b) possible metabolite schemes for the assessments with the FOCUS Surface Water models. Using SPIN, metabolite schemes for the water layer and the sediment for the FOCUS scenarios can be specified. The metabolite schemes can consist of metabolites formed in parallel or in sequence or of metabolites formed by a combination of these types.

The Access database has been replaced by a Firebird database, making the performance of TOXSWA software less dependent on versions of the operating system and versions of Microsoft Office on the computer.

Extra graphs are available via the Detailed output options.

FOCUS_TOXSWA v. 4.4.2 can also be installed on Windows 8 platforms.

Also available is TOXSWA version 1.2, which is used in the Dutch pesticide registration for first and higher-tier assessments. Higher-tier assessments include the interpretation of field studies for pesticide registration. TOXSWA v.1.2 can be downloaded via <http://www.toxswa.pesticidemodels.eu>.

1.3 Installation and registration

Official FOCUS_TOXSWA versions can be downloaded from <http://viso.ei.jrc.it/focus/>, the website of the Joint Research Centre of the EU. Notice that the installation of TOXSWA is the fourth step of the installation of the entire FOCUS surface water software package. Installation of SWASH, SPIN and

TOXSWA is explained in the read_me_first and read_me_TOXSWA text files. Installing comes down to first installing SPIN and SWASH and subsequently installing TOXSWA.

If you encounter problems in the installation of TOXSWA, contact us at

toxswa-swash@wur.nl.

FOCUS_SWASH prepares the input files for the TOXSWA model. FOCUS_TOXSWA performs all runs of a specific project and presents the main output. All input files and output files of TOXSWA are located at C:\SWASHProjects\projectname\TOXSWA, except the lateral entries input files. The lateral entries files *.m2t made by MACRO, and *.p2t made by PRZM are located at C:\SWASHProjects\projectname\MACRO\cropname, or C:\SWASHProjects\projectname\PRZM\cropname, respectively.

Users of FOCUS models can register at the JRC website in Italy.

1.4 Reporting of errors and support

Users of TOXSWA are encouraged to report difficulties and errors they experience as well as suggestions for improvements to:

toxswa-swash@wur.nl.

For errors related to running FOCUS scenarios, please contact:

focus.helpdesk@jrc.it

1.5 Documentation

This manual gives guidance for the use of FOCUS_TOXSWA 4.4.2, and provides a general description of the TOXSWA model. The theory and mathematical formulations of the pesticide processes and of the numerical solution used in TOXSWA model have been reported by Adriaanse (1996, 1997). Additionally, the effect of temperature on transformation and volatilization parameters are described in Appendix 1 by Beltman *et al.* (2006). A sensitivity analysis of the first version of TOXSWA (1.0), released in 1996, is reported by Westein *et al.* (1998). The theory and numerical solutions of the hydrology used for the FOCUS surface water scenarios are described by Adriaanse and Beltman (2009). The theory of metabolite formation in water and in sediment, and a procedure for correction of metabolite entry into FOCUS streams from their upstream catchment is described by Adriaanse *et al.* (2014). Some guidance on how to estimate input parameters for FOCUS_TOXSWA is given in Chapter 5 of Beltman *et al.* (2006).

How the use of FOCUS_TOXSWA fits in the simulation of the FOCUS surface water scenarios is documented in FOCUS (2003). Adriaanse *et al.* (2003) presented, via FOCUS_TOXSWA calculations, the effect of some FOCUS scenario assumptions on calculated exposure concentrations. TOXSWA was used to estimate degradation rates in a stagnant outdoor ditch by inverse modelling in a field study (Adriaanse *et al.*, 2013).

FOCUS_TOXSWA will often be used in combination with SWASH and SPIN. The use of SWASH is reported by Fait *et al.* (2013). A programmer's guide of SWASH is made by Te Roller *et al.* (2002). The use of SPIN is reported by Van Kraalingen *et al.* (2013).

1.6 Structure of the user manual

Chapter 2 gives an overview of the system modelled in TOXSWA and a description of the fate- related pesticide processes. Chapter 3 is the user's guide for the command line version of FOCUS_TOXSWA. The ASCII input files and the output files, made by TOXSWA during a simulation, are discussed. Chapter 4 is the users' guide for the TOXSWA Graphical User Interface. The inputs of all the windows that can be opened by the users are discussed as well as the graphs that can be generated. Chapter 5 presents example calculations for a water-sediment study and for a multi-year simulation.

2 Model description

2.1 Overview

The TOXSWA model describes the behaviour of pesticides in a water body at the edge-of-field scale, i.e. a ditch, pond or stream adjacent to a single, treated field. It calculates concentrations of pesticides and their metabolites in the water layer and in the sediment. In the water layer, the pesticide concentration varies in the horizontal direction, but is assumed to be uniform throughout its cross-sectional area. In the sediment, the pesticide concentration is a function of both horizontal and vertical directions.

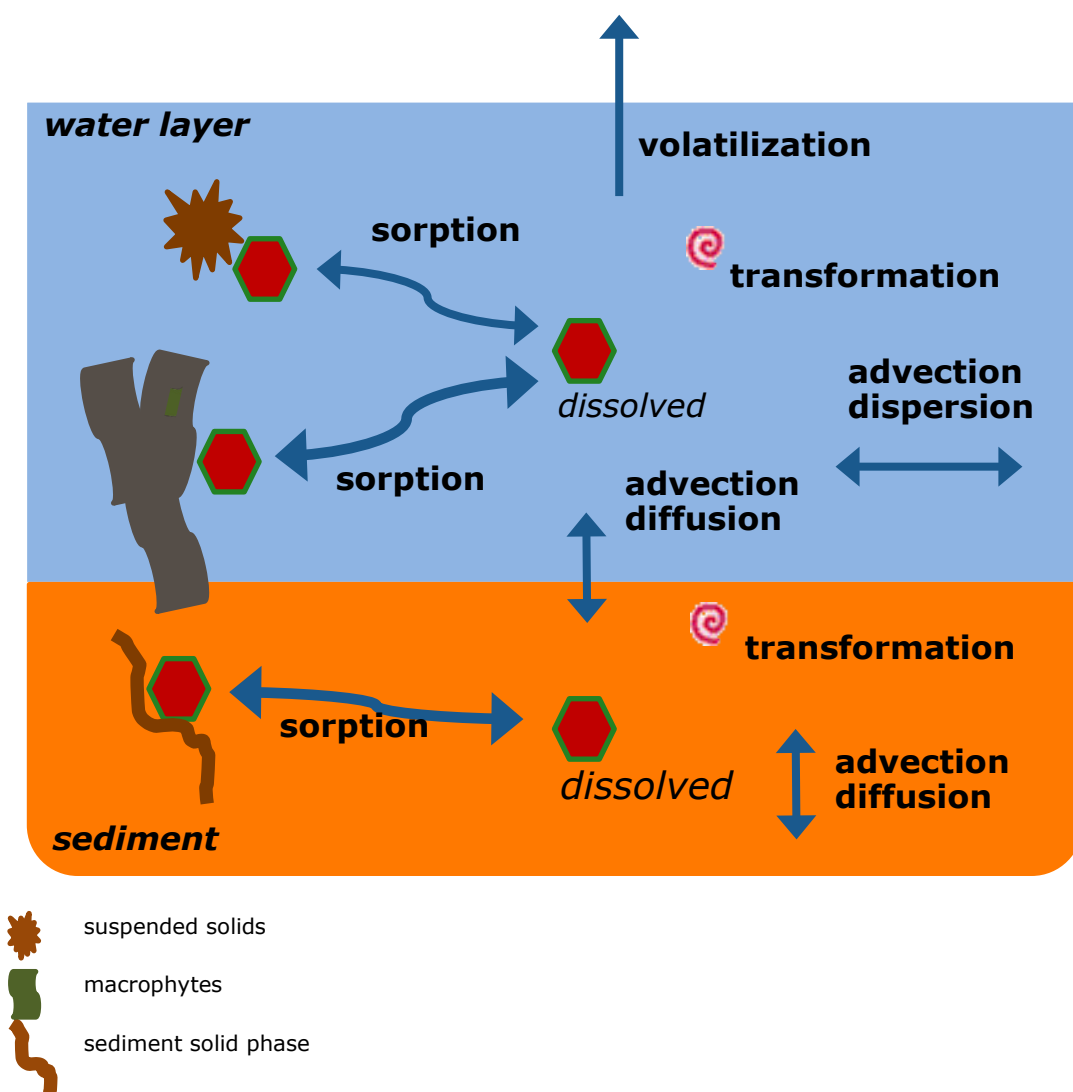


Figure 2.1 Processes in TOXSWA.

TOXSWA considers four processes: (i) transport, (ii) transformation, (iii) sorption and (iv) volatilization (Figure 2.1). In the water layer pesticides are transported by advection and dispersion, while in the sediment diffusion is included as well. Pesticides are transported across the water-sediment interface by advection (upward or downward seepage) and by diffusion. In the FOCUS surface water scenarios, transport across the water-sediment interface takes place by diffusion only. The transformation rate covers the combined effects of hydrolysis, photolysis and biodegradation. The processes transformation and volatilization are a function of temperature. Metabolite formation in water and in

sediment is modelled (see Adriaanse *et al.* 2014 for theory). Sorption to suspended solids and to sediment is described by the Freundlich isotherm. Sorption to macrophytes is described by a linear sorption isotherm but this feature is not used in the FOCUS_TOXSWA model used for the FOCUS surface water scenarios.

The simulated water body system is two-dimensional and consists of two subsystems: a water layer containing suspended solids and macrophytes and a sediment layer whose properties (porosity, organic matter content and bulk density) vary with depth. The vertical cross-section of the water subsystem has a trapezoidal shape. In the water layer subsystem, the pesticide concentration is assumed constant in the wetted cross-section, so it is only a function of the horizontal direction. In the sediment subsystem, the pesticide concentration is a function of both the horizontal and vertical directions. Water and sediment exchange pesticide mass through the wetted perimeter of the water body.

The mass balance equations for the water layer and the sediment are solved with the aid of a generalised finite-difference method. For the numerical solution, the water layer is divided into a number of nodes in the horizontal direction. Below each water layer node, an array of nodes is defined for the sediment layer (see Figure 2.2). Distances between the nodes in the water and sediment layers are in the order of magnitude of metres and millimetres, respectively.

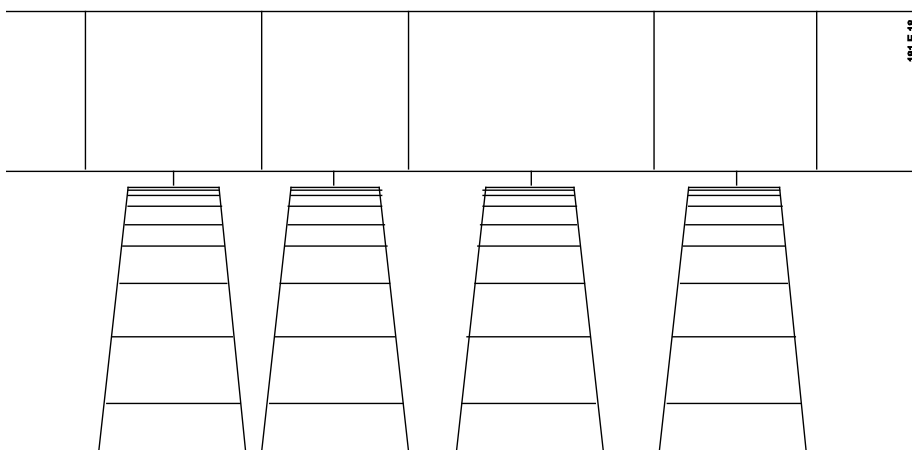


Figure 2.2 Structure of the TOXSWA water body system: one water layer subsystem and many sediment subsystems.

FOCUS_TOXSWA handles transient hydrology and water fluxes and pesticide fluxes resulting from drainage and surface runoff (including erosion), as well as instantaneous pesticide entries via spray drift deposition (Figure 2.3). In order to simulate the flow dynamics in an edge-of-field water body in a realistic way, the field-scale system is defined as the downstream part of a small catchment basin. The transient hydrology used in to model water depth and water flow is reported in Adriaanse and Beltman (2009).

The TOXSWA model does not simulate the drainage or runoff/erosion processes itself, but uses the fluxes calculated by other models as entries into the water body system of TOXSWA. For this purpose, the FOCUS_MACRO model for drainage and the FOCUS_PRZM model for runoff/erosion create output files that list the water fluxes and mass fluxes as a function of time on an hourly basis. TOXSWA uses these output files as input to calculate the hydrology and pesticide behaviour in the appropriate water body systems.

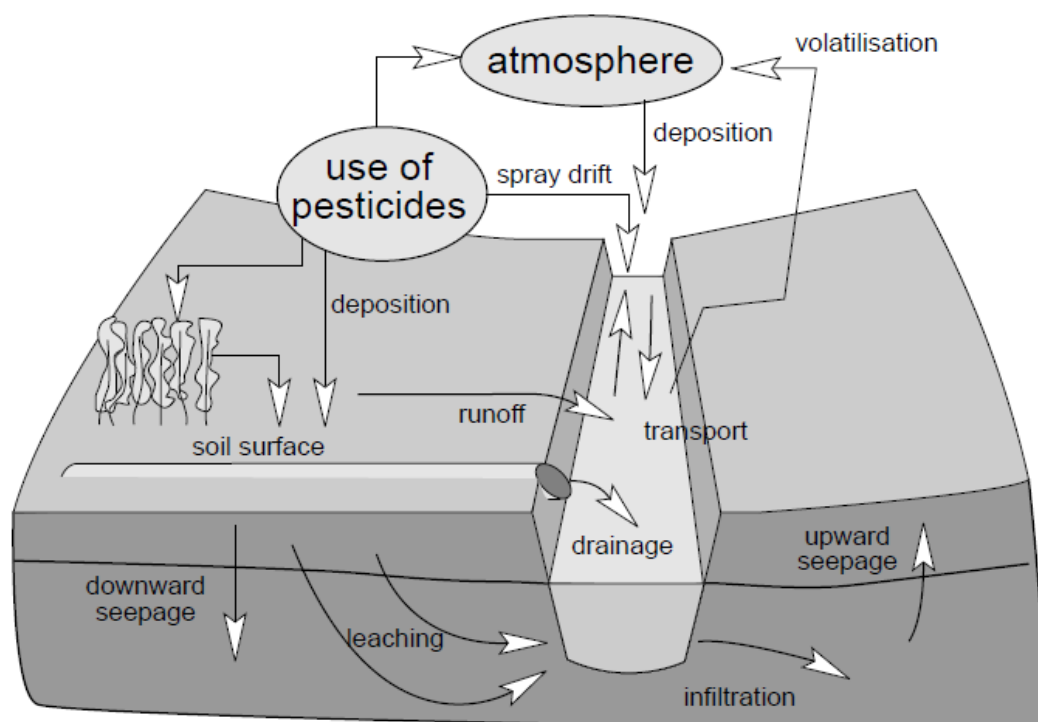


Figure 2.3 Possible entry routes of pesticides into field ditches.

2.2 Limitations

TOXSWA was developed to estimate exposure concentrations of aquatic organisms in ditches, it was not meant to simulate large water bodies like lakes or rivers. Neither is TOXSWA designed for simulations on a regional scale.

Sedimentation and resuspension are not simulated in TOXSWA, so no formation of additional sediment by sedimentation of suspended solids is simulated. The concentration suspended solids is assumed to be constant during the entire simulation period.

The sediment has been divided vertically into subsystems in the direction of flow in the watercourse (see Figure 2.2). These subsystems are composed of thin horizontal layers (segments), in which pesticide concentrations are calculated, determined by the pesticide concentrations in the overlying water layer. It has been assumed that lateral interaction between the sediment subsystems does not occur.

TOXSWA does not include the possible variation of transformation rates in time caused by e.g. changes in acidity and light intensity. In estimating the parameters for transformation, one should keep in mind which period one wants to characterise. To obtain a 24 h representative transformation rate, one may e.g., average the transformation parameters determined with and without light, weighing them for the duration of the day and night period.

It should be stressed that TOXSWA is a model, hence a simplification of reality. One should therefore always be cautious when drawing conclusions from the simulation results. Keep in mind that the quality of the model results is limited by the quality of the input data. Therefore, careful selection of the input data is of utmost importance. To verify the results of model simulations experiments can be done. When the fate of a pesticide in an experiment is simulated, accompanying experiments in the laboratory with water and sediment from the experimental site should be done to parameterize the model correctly.

3 User's guide for the command line version of FOCUS_TOXSWA

This chapter describes the command-line version of FOCUS_TOXSWA. The command-line version is of interest for those who want to use FOCUS_TOXSWA without using the User Interface. This is useful for performing FOCUS Step 4 or other higher-tier exposure calculations, uncertainty- and sensitivity analyses or inverse modelling exercises. In all other cases, we recommend the use of the FOCUS_TOXSWA Graphical User Interface (Chapter 4). This interface has some distinct advantages, such as automatic generation of input files, data-storage in a relational database, easy access to scenarios, and an integrated viewer. Please realize that the command-line version is only suitable for experienced users.

3.1 Running the model

After you have installed the model, a copy of the TOXSWA kernel (toxswa_focus_3.exe) will be available in the TOXSWA sub-folder of the SWASH folder. Copies of input files are available in the SWASH projects folder after running an example project in FOCUS_TOXSWA. It is a good practice to copy all input files to a working folder. *Do not edit the original files, so they can serve as a back-up.* The TOXSWA folder in the SWASHprojects folder contains the following two input files:

- a general input file, RunId.twx
- a meteo input file Name.met

The third input file can be found in the Macro or Przm folder of the SWASHprojects folder, depending on whether the run has a lateral entry of drainage or runoff/erosion.

- Drainage input file, RunId.m2t
- Runoff/erosion input file, RunId.p2t.

Of course, simulations should be performed with the MACRO or PRZM model before the drainage input file or runoff/erosion input files are available in the SWASHprojects folder.

You can change the name of the input files, but the extensions are fixed.

Assuming that TOXSWA is installed in the folder C:\SWASH\TOXSWA, you can start the model by typing:

```
C:\SWASH\TOXSWA\toxswa_focus_3 RunID
```

where RunID is the first part of the name of the general input file. If, for example, the name of the input file is test1.twx, you can start the TOXSWA kernel by typing:

```
C:\SWASH\TOXSWA\toxswa_focus_3 test1
```

If you wish to run the model several times, it may be handy to create a batch file "toxswa.bat", which contains the following line:

```
"C:\SWASH\TOXSWA\toxswa_focus_3" test1
```

If the batch file is put in the working directory, the model can be run by running the batch file "toxswa.bat" (e.g. by double clicking the file).

3.2 Overview of input and output files

The input for TOXSWA is organised in three input files. The files are:

RunId.twx	main TOXSWA input file
RunId.met	meteorological data
RunId.m2t or RunId.p2t	lateral entries data of respectively drainage or runoff/erosion

These files are described in the Sections 3.3 to 3.5.

The program produces three output files. The files are:

RunId.out	comprehensive output data (this file is not mandatory for registration)
RunId.sum	summary report
RunId.log	echo of main input data

The comprehensive output file is described in Sections 3.7 and the summary output file is described in Section 3.6. The file with echo of main input data is considered self-explanatory.

The program produces also two intermediate files. The files are:

RunId.hyd	hydrology data
RunId.tem	temperature data

These files are described in Section 3.8.

At the start of the simulation the RunId.WRN and RunId.ERR files are generated. If during the simulation a warning is reported, the message explaining the type of warning is written to the WRN file. If during the simulation an error occurs, the message explaining the type of error is written to the ERR file, where after the simulation stops. Normally, the simulation ends without warnings or errors. Then the WRN and ERR files are removed, and replaced by a file "toxswa.ok", indicating that the run has been finalized successfully. If warnings are given during the run (also shown during the run in the DOS-box), the WRN file remains in the folder.

Several temporary intermediate files are generated during the simulation, all with extension Name.tmp. These files are removed automatically at the end of the simulation, unless the simulation has stopped due to an error.

3.3 Description of the TOXSWA input file

3.3.1 Structure of records in the TOXSWA input file

The TOXSWA input file (see example in Annex 1) consists of obligatory and optional records. Each record contains the following fields:

- one or more fields containing the actual data,
- an obligatory field containing the identifier,
- an optional field containing the dimension of the data,
- comment fields.

The sequence of actions that are performed when an input parameters is read is described below. A flow chart illustrating the sequence of actions can be found in Tiktak *et al.* (2000, p.56).

First, the model scans the entire input file for the record containing the requested identifier. The sequence of records in the file is free. If the requested record is missing, the model either uses default values, or prints an error message. If the requested record is found, the model proceeds with verifying the dimension field. This step is followed by the actual data input. Finally, the lower- and upper

bounds of the model inputs are checked. In some cases, additional actions are undertaken: model inputs that are specified as a function of soil horizon are allocated to numerical soil layers, and model inputs that are specified in user-friendly units are converted to S.I. units as these are used within the model (i.e. g, m, mole and s). The data are echoed to the log file after conversion, so the user can check whether the model has interpreted the inputs correctly.

TOXSWA distinguishes the following type of records:

- numerical records,
- option records,
- date records,
- sediment properties,
- compound¹ properties.

Numerical records

These records are meant for single numerical values, such as the initial groundwater level. Numerical records consist of an input field (field 1), an identifier (field 2), an optional dimension field (field 3), and a comment field (rest of record). See the following example:

```
15.          ConSus    (g.m-3)    ! Concentration of suspended solids
                                   ! [1.0 - 100000]
```

Option records

Option records consist of the input field (field 1), an identifier (field 2) and a comment field (remainder of record):

```
WaterCourse  OptWaterSystemType ! Option for selecting the water system
                                   ! type (Pond, WaterCourse, Constant)
```

Date records

Date records consist of the input field (field 1), an identifier (field 2) and a comment field (remainder of record). Dates are input in the format dd-mmm-yyyy. The following month names are valid: Jan, Feb, Mar, Apr, May, Jun, Jul, Aug, Sep, Oct, Nov and Dec.

```
01-Oct-1978  TimStart           ! Start date of simulation [01-Jan-1900 -
                                   ! 31-Dec-9999]
```

Sediment properties

The input of sediment properties starts with the definition of the sediment profile in the SedimentProfile table (see Section 3.3.7). Sediment properties can then be input as a function of depth (interpolate option) or as a function of sediment horizon (horizon option). In the first case, the values specified by the user are linearly interpolated onto the numerical grid given in the SedimentProfile table. In the second case, the horizon definitions given in the table are used as a key. Sediment property tables consist of the following lines: (i) the identifier line, containing the key-word 'table', followed by the input option (horizon or interpolate), the identifier field and the dimension, (ii) the actual input records (one for each soil horizon), and (iii) the obligatory line containing the word 'end_table'. Comments between the identifier line and the end_table line are illegal:

¹ In principle to indicate a plant protection product and its metabolites the term 'substance' is used. However in the software (input and output files) the term 'compound' is used for historical reasons. Hence both terms are used in this manual, having the same meaning.

```

table horizon DispersionLength
Nr      LenDisSedLiq
      (m)
1      0.015
2      0.015
3      0.015
4      0.015
5      0.015
6      0.015
end_table

```

Multiple sediment properties can be input in one table. In this case, two extra lines are added to the header of the table. These lines contain the identifiers of the individual columns and the dimension for the individual columns. Consider the following example.

```

table horizon SedimentProperties
Nr      Rho      CntOm      ThetaSat      CofDifRel
      (kg.m-3)  (kg.kg-1)  (m3.m-3)  (-)
1      800.      0.09      0.6      0.6
2      800.      0.09      0.6      0.6
3      800.      0.09      0.6      0.6
4      800.      0.09      0.6      0.6
5      800.      0.09      0.6      0.6
6      800.      0.09      0.6      0.6
end_table

```

Compound properties

Values have to be supplied for all compounds considered in a simulation run. First, the user has to specify compound names in the compounds table (see Section 3.3.9). The records are similar to the numerical records, except that to the name of the identifier (field 2) the code of the compound is added (.e.g. _PAR, _MET1 or _MET2 in the example below).

```

100.      DT50WatRef_PAR  (d)  ! Half-life transformation in water [0.1 - 100000]
100.      DT50WatRef_MET1 (d)  ! Half-life transformation in water [0.1 - 100000]
100.      DT50WatRef_MET2 (d)  ! Half-life transformation in water [0.1 - 100000]

```

3.3.2 General rules for variable names

To improve the readability of the TOXSWA input file, a systematic approach has been followed for nomenclature of variables in the input file. Names were constructed using the three-letter codes listed in Table 3.1. These codes are usually used from left to right, and only if they are considered necessary. Sometimes several codes from one column were used, in which case they appear in alphabetical order.

Table 3.1

Notation of variable names in the TOXSWA input file.

Nature of quantity		Quantity		Process		Phase/domain		Specification	
code	description	code	description	code	description	code	description	code	description
Cof	coefficient	Ama	areic mass	Dif	diffusion	Lay	layer	App	application
Exp	exponent	Area	area	Dis	dispersion	Liq	liquid phase	Avg	average
Fac	factor	Cnt	content	Dra	drainage	Mph	macrophytes	Bal	balance
Fra	fraction	Con	concentration	Drf	drift	Om	organic matter	Bas	base
Mol	molar	Del	difference/delta	Ers	erosion	Sed	sediment	Bot	bottom
Nr	number	Dep	depth	Flo	flow	Sol	solids	Bou	boundary
Num	number	Dst	distance	Flw	flow	Sus	suspended	Cha	channel
Tim	time	DT50	transformation time 50%	For	formation	Sys	water or sediment system	Cmp	compound
		Ent	enthalpy	Hyd	hydrology	Wat	water	Cre	crest
		Flm	mass flux	Inf	infiltration			Crs	course
		Flv	volume flux	Loa	loading			Cum	cumulative
		Fre	Freundlich	Q	discharge			Dau	daughter compound
		Hgt	height	Rnf	runoff			Def	defining
		Kom	om. sorption constant	Rno	runoff			Dwn	down to

Nature of quantity	Quantity	Process	Phase/domain	Specification
	Len length	Sor sorption		End end
	Mas mass	Spg seepage		Err error
	Pre pressure	Tor tortuosity		Fld field
	Rat rate	Tra transformation		Hea energy
	Rho bulk density	Vap vaporisation		In into
	Slb solubility			Ini initial
	Tem temperature			Inp input
	Theta vol. fraction liquid			Max maximum
	Thi thickness			Met meteo
	Vel velocity			Min minimum
	Vmr volumic mass rate			Opt option
	Vol volume flux			Out out/output
	Vvr volumic volume rate			Per perimeter
				Phs physical
				Pnd pound
				Print print
				Prt parent compound
				Ref reference
				Rep representative
				Rgh roughness
				Sat saturated
				Seg segment
				Sid side
				Slo slope
				Sta start
				Stp step
				Str stream
				Sur surrounding

3.3.3 Overview of sections in the TOXSWA input file

The TOXSWA input file (`RunId.txd`) contains values for all parameters needed to execute a simulation run. In the header of the file some general information is given. The information in the header is not read by TOXSWA, so it does not affect the run. Table 3.2 gives an overview of the sections in the TOXSWA input file.

Table 3.2

Overview of sections in the TOXSWA files.

Nr	Section name	Kind of model parameters
1	Control	Simulation options
2	Waterbody	Water body properties
3	Hydrology	Hydrology properties
4	Sediment	Sediment properties
5	Weather	Weather properties
6	Compound properties	Compound properties
7	Management	Applications, loadings, and catchment factors
8	Output control	Output options

In the next eight paragraphs each of the sections is described. In Annex 2 a technical description of the TOXSWA input file is given.

3.3.4 Section 1: Control

This control section contains general options for the simulation run (see Fig. 3.1).

```
*-----
* Section 1: Control section
*-----

01-Jan-1986      TimStart      ! Start date of simulation [01-Jan-1900 - 31-Dec-9999]
30-Apr-1987      TimEnd        ! End date of simulation [01-Jan-1900 - 31-Dec-9999]
FOCUS            CallingProgram ! Calling program in FOCUS_TOXSWA for EU authorization
4               CallingProgramVersion ! Version of calling program
4               ModelVersion    ! version number of the model
4               GUIVersion      ! version number of the GUI
2               DBVersion       ! version number of the database
Hourly           OptInp         ! Option for hourly or daily input data (Hourly, Daily)
OnLine          OptHyd          ! Hydrology simulation option (Only, OnLine, OffLine,
                                ! Automatic)
OnLine          OptTem          ! Temperature simulation option (Only, OnLine, OffLine,
                                ! Automatic)
Calc            OptTimStp       ! Time step substance simulation options (Input, Calc)
600             MaxTimStpWat (s) ! Maximum calculation time step in water layer [0.001 -
                                ! 3600]
600             MaxTimStpSed (s) ! Maximum calculation time step in sediment [0.001 -
                                ! 3600]
600.            TimStpHyd (s)   ! Maximum calculation time step for hydrology [0.001 -
                                ! 3600]
No              OptScreen       ! Option to show output on screen (Yes, No)
IOMode_Full      IOMode         ! Screen output control (IOMode_Std, IOMode_Full)
```

Figure 3.1 The Control section in the TOXSWA input file.

Time domain

The time-domain for the simulation is specified with the variables `TimStart` and `TimEnd`. TOXSWA internally uses the day number since 01-Jan-1900.

Model versions

The model versions are indicated by the variables `CallingProgram`, `CallingProgramVersion`, `ModelVersion`, `GUIVersion` and `DBVersion`. The `CallingProgram` variable indicates in which context TOXSWA is used (here `FOCUS`), and by `CallingProgramVersion` which version of this context (here 4). The other variables indicate which versions model, GUI and database are used in the current context.

Input

The variable `OptInp` is used to indicate if the input is on an hourly or daily basis.

Hydrology and temperature simulation

The hydrology options (`OptHyd`) and temperature option (`OptTem`) determine how TOXSWA runs the hydrology module and the temperature module.

The following options are available:

OffLine: TOXSWA assumes that the module has already been run. The program uses an existent file that was generated in a previous runA hydrological data file (`RunId.hyd`) and/or temperature data file (`RunId.tem`).

OnLine: TOXSWA generates the data files.

Automatic: TOXSWA checks if the data file is already available. If so, the calculations hydrological, either temperature will be skipped.

Only: The hydrological module either temperature module is run, but the remainder of the simulations is skipped.

Simulation time steps

The time step variables are `TimStpHyd`, `OptTimStp`, `MaxTimStpWat` and `MaxTimStpSed`. The time step used for the simulation of the hydrology is fixed and set with `TimStpHyd`. The time step for the substance simulations (`OptTimStp`) can be input or calculated by TOXSWA. For `FOCUS` simulations the time step is calculated. When the option calculated is used the maximum time step for water

(MaxTimStpWat) and for sediment (MaxTimStpSed) can be entered. If the option OptTimStp is input, the values of the fixed time steps and the variable names TimStpWat and TimStpSed need to be given in the txw file (instead of MaxTimStpWat and MaxTimStpSed); e.g.

```
Input    OptTimStp
600.     TimStpWat
600.     TimStpSed
```

Screen output

The options OptScreen and IOMode are not operable in the FOCUS version. Hence they can be considered redundant.

3.3.5 Section 2: Water body

The Water body section specifies the dimensions of the water body and the characteristics of the water layer (see Fig 3.2).

Name and ID

The name of the location (Location) and the ID of the water body (WaterbodyID) are indicated.

```
*-----
*
* Section 2: Waterbody section
*-----
*
Rl_Stream  Location          ! Name of the location
Rl_STREAM  WaterbodyID      ! ID of the water body

* Table WaterBody
* Len          = Length (m) [0.1 - 10000]
* NumSeg       = Number of segments (-) [1 - 1000]
* WidWatSys    = Width of the bottom of water system (m) [0.1 - 100]
* SloSidWatSys = Side slope of the water system (-) [0.001 - 2]
* DepWatDefPer = Water depth defining perimeter for the exchange between water layer
*               and sediment (m) [0 - lowest water depth]

table WaterBody
Len      NumSeg    WidWatSys  SloSidWatSys  DepWatDefPer
(m)      (-)      (m)        (-)          (m)
100.     20       1.         1E-005      0.01
End_table

15.      ConSus (g.m-3)      ! Concentration of suspended solids [1.0 - 100000]
0.09     CntOmSusSol (kg.kg-1)! Mass ratio of organic matter in suspended solids [0.0 - 1.0]
0.       AmaMphWatLay (g.m-2)! Dry weight of macrophyte biomass per m2 bottom [0.0 - 1000]
```

Figure 3.2 The Water body section in the TOXSWA input file.

Water body geometry

The geometry of the water body is input through the WaterBody table. The length of the water body (Len) and the number of segments (NumSeg) used in the finite-difference scheme are provided. The cross section of the water body is defined by the width of the bottom (WidWatSys) and the side slope (SloSidWatSys). The side slope is the slope of the walls of the water body, defined as the horizontal distance divided by the vertical distance (Figure 6 in Adriaanse, 1996).

The water depth-defining perimeter (DepWatDefPer) defines the section of the side wall of the water body taken into account for exchange between water layer and sediment. It should be smaller than the water depth in the water body. Therefore, when a variable flow is simulated water depth-defining perimeter should be smaller than the lowest water level occurring in the period simulated.

TOXSWA simulates a trapezium-shaped sediment system (see Adriaanse, 1996). However, note that if the water depth defining perimeter is zero and the side slope of the water body is zero, TOXSWA simulates only the vertical column of sediment below the water layer. Such a vertical column equals the situation in artificial systems as e.g. mesocosms and water-sediment test systems (see the example in Section 5.1).

The water depth in the water body can be entered in Section 3 of the `RunId.txtw` file. It is needed when a constant flow is simulated. It is a dummy value for variable flow simulations.

Suspended solids and macrophytes

The concentration of the suspended solids (`ConSus`), its organic matter contents (`CntOmSusSol`) and the dry weight of the macrophyte biomass per m² water body bottom (`AmaMphWatLay`) have to be entered.

3.3.6 Section 3: Hydrology

The Hydrology section specifies the type of hydrology of the water body, and the parameterisation of the selected hydrology type (see Figure 3.3). For the FOCUS ditches and streams hydrology is simulated using transient water flow. Background information on the transient water flow module of TOXSWA can be found in Adriaanse and Beltman (2009).

```
*-----
*
* Section 3: Hydrology: general
*-----
*
WaterCourse   OptWaterSystemType   ! Option for selecting the water system type
Variable      OptFloWat             ! (Pond, WaterCourse, Constant)
                                     ! Option for water flow (Constant, Variable)

* if: OptWaterSystemType = WaterCourse
Fischer       OptDis                ! Options are 'Fischer' and 'Input'

* if: OptDis = Input
0.            CofDisPhsInp (m2.d-1) ! Dispersion coefficient [0. - 100000]
*-----
*
* Section 3a: Constant water flow
*-----
*
* if: OptFloWat = Constant
1.            DepWat (m)
0.            VelWatFlwBas (m.d-1)
*-----
*
* Section 3b: Variable water flow: pond
*-----
*
* if: OptFloWat = Variable and OptWaterSystemType = Pond
0.45          AreaSurPndInp (ha)    ! Size of area surrounding the pond [0.0 - 50.0]

* if: CallingProgram = FOCUS
3.189         QBasPndInp (m3.d-1)   ! Base flow, i.e. inflow into pond [0.001 - 50.0]
1.            HgtCrePnd (m)         ! Height of the weir crest [0.1 - 5.0]
0.5           WldCrePnd (m)         ! Width of the weir crest [0.01 - 10]

* if: Opt = Runoff
0.06          AreaErsSurPndInp (ha) ! Size of the eroding area around the pond [0.0 - 50.0]
*-----
*
* Section 3c: Variable water flow: watercourse
*-----
*
* if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
*representative channel
0.001         SloBotRepCha (-)      ! Slope bottom representative channel [0.0 - 0.01]
0.5           HgtCreRepCha (m)      ! Height of the weir crest [0.1 - 5.0]
0.5           WldCreRepCha (m)      ! Width of the weir crest [0.01 - 10]

110.          LenRepCha (m)         ! Length representative channel [10.0 - 2000]
1.            WidBotRepCha (m)      ! Width bottom representative channel [0.1 - 10]
1E-005        SloSidRepCha (-)     ! Side slope of the representative channel [1.0 - 100]

11.           CofRghRef (-)         ! Value of the Manning coefficient for bottom roughness
                                     ! [1.0 - 100]
1.2           CofVelHea (-)         ! Energy coefficient resulting from the non-uniform
                                     ! distribution of flow velocities [1.1 - 1.5]

* if: CallingProgram = NL or FOCUS
100.          AreaUpsWatCrsInp (ha) ! Size of the area upstream the representative channel
                                     ! [0.0 - 10000]
191.8         QBasWatCrsInp (m3.d-1) ! Minimal flow into watercourse [0.0 - 10000]

100.          AreaUpStrRepCha (ha)  ! Size of the area upstream the representative channel
                                     ! [0.0 - 10000]
191.8         QBasRepCha (m3.d-1)   ! Minimal flow into watercourse [0.0 - 10000]
```

Figure 3.3 The Hydrology section in the TOXSWA input file.

Definition of water flow, water body type and dispersion

The type of water flow (`OptFloWat`) can be either `Constant` or `Variable`. Also the type of water body (`OptWaterSystemType`) must be provided; a `Pond`, consisting of one single segment in the water layer, or a `WaterCourse`, consisting of more than one segment in the water layer.

TOXSWA uses only those parameters that concern- the selected options i.e. in Section 3a Constant water flow (pond and watercourse), in Section 3b Variable water flow in a pond, and in Section 3c Variable water flow in watercourse. The parameters in the sections not relevant for the chosen options (`OptFloWat`, `OptWaterSystemType`) will not be used by TOXSWA.

The watercourses of the FOCUS surface water scenarios are either ditches or streams, depending on the characteristics determining the flow, like bottom slope and size of water fluxes that enter the watercourse. In order to simulate variable flow in a watercourse in a realistic way, the field-scale system is defined as the downstream part of a small catchment basin. Therefore additional parameters describe this system.

In waterbodies consisting of one segment in the water layer (ponds) longitudinal dispersion is not calculated. For watercourses the dispersion is taken into account. The option `OptDis` indicates using an Input value, or calculation the dispersion coefficient according to Fischer. When the option Input is selected a value for the dispersion coefficient must be entered (`CofDisPhsInp`).

Constant flow (Section 3a)

The constant water depth in the water body (`DepWat`) and the constant flow velocity (`VelWatFlwBas`) in the pond or in the watercourse need to be entered.

Variable flow in a pond (Section 3b)

The area around the pond that contributes water and pesticide fluxes to the pond is defined by `AreaSurPndInp`. If runoff is the lateral entry route the area `AreaErsSurPndInp` contributes pesticide fluxes by erosion. The fluxes in the drainage or runoff files (indicated in Section 7) are multiplied by these areas to simulate the water and mass fluxes entering the pond. Next to these water and erosion fluxes the base flow `QBasPndInp` that continuously enters the pond has to be specified. The height of the weir in the pond up to its crest `HgtCrePnd` and the crest width of the weir `WidCrePnd` control the outflow of the pond.

Variable flow in a watercourse (Section 3c)

Depending on its flow regime and hydromorphic properties, the watercourses of the FOCUS surface water scenarios resemble a ditch or a stream. The water fluxes used in the mass balance calculations are based on a water balance for TOXSWA's watercourse. This water balance accounts for all incoming and outgoing water fluxes of the watercourse. Within a time step, a constant water depth is assumed for the whole watercourse. In the representative channel calculation, this constant water depth is determined as a function of time. The representative channel represents the average conditions in the catchment considered. It is defined by a length, `LenRepCha`, a bottom slope, `SloBotRepCha`, a bottom width, `WidBotRepCha`, and a side slope, `SloSidRepCha`. Its inflow is composed of a small, constant base flow, `QBasRepCha`, and either the runoff or the drainage fluxes from the upstream catchment with area `AreaUpStrRepCha`. As both runoff and macropore flow to drains are event-driven processes, discharges and water levels may be very dynamic. A minimum water depth, occurring during low base flows, needs to be maintained with the aid of a weir in the representative channel. The weir is defined by the height of its crest, `HgtCreRepCha`, and the width of its crest, `WidCreRepCha`. The flow conditions are calculated with the aid of the Chézy-Manning equation for a backwater curve in front of a weir, or for uniform flow conditions (if the influence of the weir is no longer noticeable, because it is located far downstream). For these calculations the Manning coefficient, describing the bottom roughness, `CofRghRef`, and an energy coefficient resulting from the non-uniform distribution of flow velocities, `CofVelHea`, are also needed. The calculated water depth at the upstream end of the representative channel is a function of time. This $h(t)$ is assumed to be the water depth for TOXSWA's watercourse over its entire length, and is used in the water balance calculations.

TOXSWA's watercourse is defined by the water body parameters of Section 2; its base flow from the upstream catchment, `QBasWatCrsInp`, and the size of the upstream area delivering drainage or runoff fluxes into the watercourse, `AreaUpsWatCrsInp`, need to be specified.

3.3.7 Section 4: Sediment

In this section, the sediment profile, vertical discretization and sediment properties have to be specified (see Figure 3.4).

ID

The ID of the sediment type (`SedimentTypeID`) is indicated.

Sediment profile

The vertical discretization of the sediment layer is input through the `SedimentProfile` table. For each sediment horizon, the thickness of the horizon (`ThiHor`), and the number of sediment layers (`NumLay`) used in the finite-difference scheme (see Figure 18 in Adriaanse, 1996) must be provided. The number of sediment layers is a compromise between accuracy and computation time. Computation time increases approximately with the square of the number of sediment layers. On the other hand, predictions may become inaccurate if the segment thickness is taken too large. Furthermore, then mass balance errors may become too large. For most simulations, however, a segment-thickness of 1 to 2 mm in the top 0.01 m, 5 – 10 mm in the 0.01 – 0.05 m sediment layers and 20 and 30 mm for the layers below 0.05 m is a fair compromise.

Sediment properties

If `OptSedimentProperties` is set to `Input`, the porosity and relative diffusion coefficient should be provided in the table `SedimentProperties`. If these are unknown, they can be calculated by TOXSWA. If `OptSedimentProperties` is set to `Calc`, the model calculates the porosity (ε , `ThetaSat`) from the dry bulk density (ρ_d , `Rho`), the phase densities of organic matter (ρ_{om} in kg L^{-1}) and of mineral matter (ρ_{min} in kg L^{-1}), and the organic matter content (m_{om} , `CntOm`):

$$\varepsilon = 1 - \frac{\rho_d}{\rho_{om}} m_{om} - \frac{(1 - m_{om}) \rho_d}{\rho_{min}} \quad (1)$$

This equation states that the volume fractions of water, organic matter and mineral parts sum up to 1 (Koorevaar *et al.*, 1983). Phase densities that can be used are 1.40 kg L^{-1} for ρ_{om} and 2.65 kg L^{-1} for ρ_{min} (Koorevaar *et al.*, 1983). Note that the phase densities are based on soils, and not on sediment. The phase density of organic matter may be too high for sediment. Because data for sediment is not available the soil values are used. To calculate the relative diffusion coefficient (λ , `CofDifRel`) the model uses:

$$\lambda = \frac{1}{1 - \ln(\varepsilon^2)} \quad (2)$$

Eq. (2) is an empirical equation derived by Boudreau (1996) on the basis of experiments on sediments and combined with theoretical work (see also Annex 6).

Basic sediment properties are input in the `SedimentProperties` table. For each sediment horizon (`Nr`), the dry bulk density (`Rho`), the mass content of organic matter (`CntOm`), the porosity (`ThetaSat`) and the relative diffusion coefficient (`CofDifRel`) need to be specified. In case `OptSedimentProperties` is set to `Calc` values inserted for `ThetaSat` and `CofDifRel` are dummy values. The mass content of organic matter refers to dry sediment. The diffusion of substances is affected by the diffusion coefficient in water and by the relative diffusion coefficient. The diffusion coefficient is a substance property. The relative diffusion coefficient (also called tortuosity) is a sediment layer property.

Seepage and dispersion length

A constant seepage/infiltration flow (`FlwWatSpg`) from the contributing plot into the water body (negative values) or out of the water body (positive values) can be entered. For upward seepage (negative values), the concentration in the seeping water (`ConWatSpg`) needs to be specified in Section 7. If the seepage/infiltration flow is not zero the dispersion length, `LenDisSedLiq`, should be

given for each sediment horizon (table DispersionLength). Note that seepage is zero in FOCUS scenarios, so the dispersion table is not needed in the input file.

Erosion

If the lateral entry is occurring via runoff and erosion (i.e. OptLoa = PRZM, see Section 3.5), pesticide mass sorbed onto the eroded soil that enters the water body will be added to the top of the sediment (specified by ThiLayErs). The pesticide mass is evenly distributed in this top layer of the sediment. The eroded soil itself is not accounted for (i.e. the sediment mass is not increased by eroded soil particles).

```
*-----
*
* Section 4: Sediment section
*-----
*
FOCUS      SedimentTypeID  ! Name of sediment type

* table SedimentProfile
* ThiHor = thickness of horizon []
* NumLay = number of layers in horizon [1,]

table SedimentProfile
ThiHor    NumLay
(m)
0.004      4
0.006      3
0.01       2
0.03       3
0.02       1
0.03       1
end_table

Input      OptSedProperties  ! Option sediment properties [Input, Calc]

* table specifying SedimentProperties for each horizon:
* Nr       = number horizon []
* Rho      = bulk density [100 - 2000]
* CntOm    = organic matter mass content [0.1 - 1.0]
* ThetaSat = saturated water content [0.1 - 0.95]
* CofDifRel = relative diffusion coefficient [0.0 - 1.0]

table horizon SedimentProperties
Nr      Rho      CntOm    ThetaSat  CofDifRel
        (kg.m-3) (kg.kg-1) (m3.m-3)  (-)
1       800.     0.09     0.6       0.6
2       800.     0.09     0.6       0.6
3       800.     0.09     0.6       0.6
4       800.     0.09     0.6       0.6
5       800.     0.09     0.6       0.6
6       800.     0.09     0.6       0.6
end_table

0.          FlwWatSpg (m3.m-2.d-1)

* If: FlwWatSpg not zero
* table horizon DispersionLength
* Nr       = Horizon number []
* LenDisSedLiq = Dispersion length of solute in liquid phase [0.05 - 1.0]

table horizon DispersionLength
Nr      LenDisSedLiq
        (m)
1       0.015
2       0.015
3       0.015
4       0.015
5       0.015
6       0.015
end_table

* If: OptLoa = PRZM
0.01     ThiLayErs (m)      ! Thickness of sediment layer to which eroded soil is added
```

Figure 3.4 The Sediment section in the TOXSWA input file.

3.3.8 Section 5: Weather

The Weather section specifies weather data (see Fig 3.5). The name of the file with weather data (MeteoStation) must be specified. The format of the file with weather data is described in Section 3.4. The type of input, i.e. Hourly, Daily or Monthly needs to be indicated (OptMetInp).

```

*-----
*
* Section 5: Weather section
*-----
*

Weiherbach      MeteoStation  ! Name of the *.met file with meteo data

Monthly         OptMetInp      ! Option for input data (Hourly, Daily, Monthly)

```

Figure 3.5 The Weather section in the TOXSWA input file.

3.3.9 Section 6: Compound properties

The Compound section lists the properties of all compounds (see Fig. 3.6). In this section of the TOXSWA input file, the identifier names are concatenated with compound names (in this example EXSW2). The maximum length of each code is six letters.

Compounds and metabolite schemes

The compounds section starts with the name of the parent compound (*SubstanceName*). Then a list of compound codes of all compounds in the simulation should be entered in the `table compounds`.

The transformation scheme for compounds formed in water (see also Fig. 3.6) is input in the `table FraPrtDauWat`. For each parent compound, the molar fraction of compound transformed into a daughter must be specified. Figure 3.6 shows an example for three transformations; the parent compound EXSW2 is for 70% transformed into the daughter MetW1. This daughter MetW1 is for 100% transformed into a consecutive daughter MetWa2. Next to the parent also a metabolite formed in soil MetSol enters the water body, which is for 50% transformed into daughter MetWa2. For transformations in sediment the compounds and formation fractions must be entered similarly in `table FraPrtDauSed`.

Molar mass

The molar mass (*MolMas*) must be specified.

Transformation

The DegT50 of the compound in the water layer (*DT50WatRef*) and the temperature at which it is measured (*TemRefTraWat*) have to be entered. The molar activation enthalpy (*MolEntTraWat*) adapts the transformation rate in water from the observed temperature to the rate at the temperature of the system (temperatures based on entry from *RunId.met* file, see Section 3.4). In addition, the DegT50 of the compound in the sediment layer (*DT50SedRef*) and the temperature at which it is measured (*TemRefTraSed*) and molar activation enthalpy in sediment (*MolEntTraSed*) need to be specified.

Sorption

The sorption of compounds is described with Freundlich-type isotherms. The slope of the Freundlich-type isotherm for sorption to suspended solids is based on the organic matter content, *KomSusSol*, and curvature by the Freundlich exponent for sorption to suspended solids, *ExpFreSusSol*. The value of the reference concentration must be introduced in the *ConLiqRefSusSol* record. Its value must be within the concentration range of the simulation study. The default value is 1 mg L⁻¹. The Freundlich isotherm for sorption is used for the sediment as well. So, the same parameters as above, but then applying to the sediment; *KomSed*, *ExpFreSed* and *ConLiqRefSed*, have to be entered. The slope of the linear isotherm for sorption of the pesticide to macrophytes, *CofSorMph*, has to be entered as well.

Volatilization

The saturated vapour pressure (*PreVapRef*), the temperature at which it is measured (*TemRefVap*) and the molar enthalpy of vaporisation (*MolEntVap*), needed to calculate the saturated vapour pressure at other temperatures, have to be entered. Likewise, the solubility (*SlbWatRef*),

temperature at which the solubility is measured (TemRefSlb) and molar enthalpy of solubility (MolEntSlb) have to be specified.

Diffusion coefficient

The diffusion coefficient of pesticides in pure water (CofDifWatRef) is a compound property and must be specified in this section. The relative diffusion coefficient is specified in the sediment section (Section 3.3.7).

```
*-----
*
* Section 6: Compound section
*-----
*
EXSW2      SubstanceName      ! Name of parent substance [1 - 6 characters]

table compounds                ! List of substances [1 - 6 characters]
EXSW2
end_table

* Table parent-daughter relationships transformation in water (FraPrtDauWat):
* Column 1: fraction formed from parent into daughter
* Column 2: name of parent
* Column 3: name of daughter

table FraPrtDauWat (mol.mol-1)
0.7 EXSW2 -> MetW1
1.0 MetW1 -> MetW2
0.5 MetSol -> MetW2
end_table

* Table parent-daughter relationships transformation in sediment (FraPrtDauSed):
* Column 1: fraction formed from parent into daughter
* Column 2: name of parent
* Column 3: name of daughter

Table FraPrtDauSed (mol.mol-1)
end_table

* Substance properties for each substance given in table compounds
* Substance code is extension of parameter name
*----- Parent: EXSW2 -----

300.      MolMas_EXSW2 (g.mol-1) ! Molar mass of parent substance [10.0 - 10000]

100.      DT50WatRef_EXSW2 (d)   ! Half-life transformation in water [0.1 - 100000]
20.      TemRefTraWat_EXSW2 (C) ! Temperature at which half-life was measured [5.0 - 30]
65.4     MolEntTraWat_EXSW2 (kJ.mol-1) ! Molar activation enthalpy of transformation in
! water [0.0 - 200]

300.      DT50SedRef_EXSW2 (d)   ! Half-life transformation in sediment [0.1 - 100000]
20.      TemRefTraSed_EXSW2 (C) ! Temperature at which half-life was measured [5.0 - 30]
65.4     MolEntTraSed_EXSW2 (kJ.mol-1) ! Molar activation enthalpy of transformation in
! sediment [0.0 - 200]

58.      KomSed_EXSW2 (L.kg-1)  ! Coefficient of equilibrium sorption in sediment
! [0.0 - 10000000]
1.      ConLiqRefSed_EXSW2 (mg.L-1) ! Reference concentration in liquid phase in
! sediment [0.001 - 100]
1.      ExpFreSed_EXSW2 (-)     ! Freundlich exponent in sediment [0.1 - 2]
58.      KomSusSol_EXSW2 (L.kg-1) ! Coefficient of equilibrium sorption suspended
! solids [0.0 - 10000000]
1.      ConLiqRefSusSol_EXSW2 (mg.L-1) ! Reference concentration in liquid phase
! suspended solids [0.001 - 100]
1.      ExpFreSusSol_EXSW2 (-)  ! Freundlich exponent suspended solids [0.1 - 2]

0.      CofSorMph_EXSW2 (L.kg-1) ! Coefficient for linear sorption on macrophytes
! [0.0 - 20000]

1.E-7    PreVapRef_EXSW2 (Pa)   ! Saturated vapour pressure [0.0 - 200000]
20.      TemRefVap_EXSW2 (C)    ! Temperature of reference at which the saturated vapour
! pressure was measured [0.0 - 40]
95.      MolEntVap_EXSW2 (kJ.mol-1) ! Molar enthalpy of the vaporization process
! [-200 - 200]

1.      SlbWatRef_EXSW2 (mg.L-1) ! Water solubility [0.001 - 1000000]
20.      TemRefSlb_EXSW2 (C)    ! Temperature of reference at which the water solubility
! was measured [0.0 - 40]
27.      MolEntSlb_EXSW2 (kJ.mol-1) ! Molar enthalpy of the dissolution [-200 - 200]
4.3E-5   CofDifWatRef_EXSW2 (m2.d-1) ! Reference diffusion coefficient in water
! [0.0 - 200]
```

Figure 3.6 The Compound section in the TOXSWA input file.

3.3.10 Section 7: Management

The Management section concerns loadings (spray drift, drainage, and runoff) into the water body, upstream catchment options and initial and boundary concentrations (see Fig. 3.7).

The name of the application scheme (`ApplicationScheme`) is indicated.

Loading option

One of the five options for the type of loading, `OptLoa`, must be selected. Note that drainage and runoff cannot be simulated simultaneously by TOXSWA in the current version. Only one of these loading types can be selected.

Spray drift and stretch of the water body where loadings enter

In the `Table loadings` the spray drift loadings are defined. For each loading, the date, the type of loading (default `drift`), drift deposited at the water surface, the start of the stretch of the watercourse to which loadings are added and the end of this stretch have to be specified. The loadings should be entered in chronological order. For runs comprising drainage or runoff loadings, the dates are dummy values, because the application dates reported in the headers of the drainage or runoff files overrule the dates in the `RunId.txd` file. Furthermore, the start distance and the end distance of the stretch of the water body is used for all entries, hence also for drainage and for runoff. The drift deposition can be calculated from the spray drift percentage and the application rate with:

$$\text{drift deposition (mg m}^{-2}\text{)} = \frac{\text{spray drift (\%)}}{100} \cdot \frac{\text{application rate (g ha}^{-1}\text{)}}{10} \quad (3)$$

Drainage and runoff loadings

When drainage or runoff is to be simulated the path and name of the files with drainage or runoff fluxes need to be indicated in the `table Soil substance files`. If a metabolite formed in soil is entering the water body, the path and name of the file need to be in this table also.

If drainage is simulated, i.e. PEARL or MACRO has been selected as loading option, the width of the field contributing drainage, `WidFldDra`, needs to be entered.

If runoff is simulated, i.e. PRZM has been selected as loading option, the width of the field contributing runoff, `WidFldRnf`, the width of the field contributing erosion, `WidFldErs`, and the ratio of infiltration water added to runoff water, `RatInfDir`, need to be entered. Next to runoff water flowing over the soil, part of the infiltrating water enters the water body through the soil. This part of the infiltration flux is calculated via multiplication of `RatInfDir` with the infiltration flux given in the runoff output file of PRZM. Pesticides do not enter the water layer via this indirect route. Apart from pesticide entries in runoff water, also pesticides adsorbed to eroded soil enter the water body. This pesticide mass is added into an upper layer of the sediment as defined by `ThiLayErs` (see Section 3.3.7).

Upstream catchment

For watercourses, pesticide fluxes from the upstream area are simulated by turning on the switch `OptUpsInp`. If `OptUpsInp` is `Yes` the ratio of the upstream area treated with pesticide, `RatAreaUpsApp`, should be entered. TOXSWA calculates the mass entering via the upstream boundary by multiplying this ratio `RatAreaUpsApp` with the area of the upstream catchment `AreaUpsWatCrsInp` (see Section 3.3.6) and the pesticide flux read from the drainage or runoff file. This entry across the upstream boundary occurs simultaneously with the lateral inputs. There is no delay by transport of water or pesticide in the catchment. For runoff simulations, the entry of pesticide mass adsorbed to eroded soil via the upstream boundary is not taken into account.

Metabolite formation in water in upstream catchment

If metabolites are formed in water a correction factor for metabolite formation in the upstream catchment, $CF_{m,up}$ (`FraMetForUps`), needs to be entered. This correction factor is used for the fraction metabolite formed in water from mass deposited by spray drift on surface waters in the upstream catchment, and for the fraction metabolite formed in water from mass originated from drainage or runoff into surface waters in the upstream catchment. See Adriaanse *et al.* (2014) for the theoretical basis of this correction factor and the procedure to calculate this correction factor. The default value is 1, indicating a formation fraction of 1.0 of the parent.

Concentration in air

TOXSWA uses the concentration in the air (ConAir) to determine the concentration gradient between the water phase and the atmosphere in order to calculate the volatilisation through the water surface. In the absence of data, we generally select the concentration in the air to be zero.

Concentration in seepage water

If seepage is not zero (see Section 3.3.6) and the seepage is upward in the water body (negative values) the concentration in the seeping water (ConWatSpg) can be specified.

Initial concentration in water

The initial concentration of the parent in the water layer ConSysWatIni has to be entered (default is 0.0). This is the total concentration (c^*), so including mass adsorbed to suspended solids. The initial concentration of metabolites cannot be specified.

Initial mass content in sediment

The initial mass content of the parent in sediment can be entered in the table CntSysSedIni. Note that this initial content represents the total content of pesticide present, i.e. in the solid phase and in the liquid phase of the sediment. The entered contents are used for each sediment subsystem, hence along the whole length of the water body. The initial mass content of metabolites cannot be specified.

```
*-----
*
* Section 7: Management section
*-----
*
* Loading options (OptLoa):
* DriftOnly = spray drift only entry route
* PEARL      = drainage calculated by PEARL
* MACRO      = drainage calculated by MACRO
* PRZM       = runoff and erosion calculated by PRZM
* GEM        = point source calculated by GEM
*
MACRO      OptLoa      ! Loading options (DriftOnly, PEARL, MACRO, PRZM, GEM)
FOCUS_EXAMPLE ApplicationScheme ! Name of the application scheme
*
* Table loadings
* Column 1: Date of application, relevant if OptLoa = DriftOnly, otherwise the date
*           is a dummy values
* Column 2: Type of loading (-)
* Column 3: Drift deposition (mg.m-2) []
* Column 4: Start of stretch of watercourse loaded by all loading types (m) []
* Column 5: End of stretch of watercourse loaded by all loading types (m) []
*
table Loadings
30-Dec-1899  drift      0.154      0.      30.
30-Dec-1899  drift      0.1155     0.      30.
30-Dec-1899  drift      0.077      0.      30.
end_table
*
* If: OptLoa = MACRO or OptLoa = PRZM
* Table with path+name of lateral entries files
table Soil substance files
C:\SwashProjects\project_EXSW2\MACRO\cereals_winter\macro00001_p.m2t
end_table
*
* If: OptLoa = PEARL or OptLoa = MACRO
0.      WidFldDra (m)      ! Width of field contributing drainage
*
* If: OptLoa = PRZM
0.      WidFldRnf (m)      ! Width of field contributing runoff
0.      WidFldErs (m)      ! Width of field contributing erosion
0.      RatInfDir (-)      ! Ratio of infiltration water added to runoff water
*
* If: CallingProgram = FOCUS and OptWaterSystemType = WaterCourse
Yes      OptUpsInp      ! Switch for upstream catchment treated (Yes, No)
0.      RatAreaUpsApp (-) ! Ratio of upstream catchment treated [0.0 - 1]
1.      FraMetForDrfUps (-) ! Fraction primary metabolites formed in water
                                ! in upstream catchment [0.0 - 1]
0.      ConAir (kg.m-3)    ! Concentration of the substance in air
0.      ConWatSpg (g.m-3)  ! Concentration in incoming seepage water
0.      ConSysWatIni (g.m-3)
*
* Table initial substance content in sediment (CntSysSedIni)
* Column 1: Depth in sediment (m)
* Column 2: Substance content (mg.kg-1)
table interpolate CntSysSedIni (mg.kg-1)
end_table
```

Figure 3.7 The Management section in the TOXSWA input file.

3.3.11 Section 8: Output control

In this section, the output of TOXSWA is controlled (see Fig. 3.8).

Remove RunId.out file

It is possible to specify whether the output file should be saved. If `OptDelOutput` is set to `Yes`, the output file will be removed. This option saves run time and is thus useful if summary information is required only.

Reports

Specify the desired report type via `OptReport`, and indicate if the `PercentileReport` is needed. The `PercentileReport` is not available for FOCUS simulations.

Formats

Specify the desired format of the date (`DateFormat`) and the actual values in the output file (`OutputFormat`). The `DateFormat` can be set to `DaysFromSta` (print the number of days since the start of the simulation), `DaysFrom1900` (print the number of days since 1-Jan-1900) or `Years` (print the number of years since the start of the simulation). To specify the output format of the reals (`RealFormat`), standard FORTRAN notation should be used.

Target layer in sediment

The thickness of the target layer (`ThiLayTgt`) is input. The exposure concentrations in sediment are calculated as the average concentration in this layer.

Output

With `OptDelTimPrn` the output time step is set. Specify the desired (fixed) output interval (`DelTimPrn`). If set to zero, TOXSWA will calculate the output interval based on begin and end date of the simulation. It is important to realize that TOXSWA generates averages over the print interval and not point values. This implies that a larger print interval generates a smoother pattern of resulting values (because calculated values are averaged over a longer period). If `OptDelTimPrn` is `Other`, the time step is set with `DelTimPrn`. Specify whether fluxes should be cumulated over the entire simulation period (`PrintCumulatives`).

Distances and depths

An option for the output of the variables in the water layer (`OptOutputDistances`) must be selected. If `Table` is selected in the table `OutputDistances` the distances for which output is requested can be specified. Then the concentration at the middle of the segment that is closest to the requested distance is given.

In the table `OutputDepths` can be specified for which depths in sediment output is requested. Then the concentration at the middle of the segment that is closest to the requested depth is given.

Horizontal profiles

The user can specify a number of dates at which horizontal profiles of the most important state variables in the water layer are produced (table `HorizontalProfiles`).

Print variables

Specify for each variable whether output is wanted or not (`print_`).

```

*-----
*
* Section 8: Output control
*-----
*
No          OptDelOutFiles  ! Switch for removing *.out files after run (Yes, No)
FOCUS       OptReport      ! Options for report type (DutchRegistration, FOCUS)
Yes         ExposureReport ! Exposure report (Yes, No)
No          PercentileReport ! Percentile report (Yes, No)
DaysFromSta DateFormat    ! Date format (DaysFromSta, DaysFrom1900, Years)
el4.6       RealFormat     ! Number format of the reals

0.05        ThiLayTgt (m)  ! Thickness of the target layer
Hour        OptDelTimPrn   ! Option to set output time step (Hour, Day, Decade,
                        ! Month, Year, Automatic, Other)
1           DelTimPrn (d)  ! Output time step [0.0 - length simulation period]
No          PrintCumulatives ! Specify whether fluxes should be cumulated over the
                        ! entire simulation period (Yes, No)

* table HorizontalProfiles: dates are given for which detailed output is wished
* Column 1: dates
table HorizontalProfiles
end_table

* Table output depths (OutputDepths): indicate for which depths the output is selected
* Column 1: Depth
table OutputDepths (m)
end_table

All OptOutputDistances          ! Switch output distances (None, All, Table)

* Table output distances (OutputDistances): indicate for which distance the output is
* selected
* Column 1: Distance
table OutputDistances (m)
end_table

No      print_VelWatFlw      ! Flow velocity (m/h) [Yes, No]
Yes     print_QBou          ! Discharge (m3/h) [Yes, No]
Yes     print_VvrLiqDra     ! Drain flow (m/h) [Yes, No]
Yes     print_VvrLiqRnf     ! Runoff flow [Yes, No]
Yes     print_FlmDra        ! Drain substance flux [Yes, No]
Yes     print_FlmRnf        ! Runoff substance flux [Yes, No]
Yes     print_FlmErs        ! Erosion substance flux [Yes, No]
Yes     print_ConLiqWatLay  ! Concentration in water, hour average (g/m3) [Yes, No]
Yes     print_ConSysWatLay  ! Total concentration in water (g/m3) [Yes, No]
Yes     print_CntSorMph     ! Content sorbed to macrophytes [Yes, No]
Yes     print_CntSorSusSol  ! Content sorbed suspended solids [Yes, No]
Yes     print_ConSysSed     ! Total content in sediment [Yes, No]
Yes     print_ConLiqSed     ! Concentration in pore water sediment (g/m3) [Yes, No]
Yes     print_CntSorSed     ! Content sorbed to sediment [Yes, No]
Yes     print_DepWat        ! Water depth (m) [Yes, No]
No      print_DepWatRepCha  ! Water depth representative channel [Yes, No]
Yes     print_CntSedTgt     ! Total content in target layer sediment [Yes, No]
Yes     print_ConLiqSedTgt  ! Concentration in pore water in target layer sediment [Yes, No]
Yes     print_CntSorSedTgt  ! Content sorbed in target layer sediment [Yes, No]
Yes     print_ConLiqWatLayCur ! Concentration in water, at end hour (g/m3) [Yes, No]
Yes     print_AmaWatLay     ! Mass in water layer [Yes, No]
Yes     print_AmaLiqWatLay  ! Mass in liquid phase in water layer [Yes, No]
Yes     print_AmaSorSusSol  ! Mass sorbed to suspended solids in water layer [Yes, No]
Yes     print_AmaSorMph     ! Mass sorbed to macrophytes in water layer [Yes, No]
Yes     print_AmaSed        ! Mass in sediment layer [Yes, No]
Yes     print_AmaLiqSed     ! Mass in liquid phase in sediment layer [Yes, No]
Yes     print_AmaSorSed     ! Mass sorbed in sediment layer [Yes, No]
Yes     print_AmaTraWatLay  ! Mass transformed in water layer [Yes, No]
Yes     print_AmaForWatLay  ! Mass formed in water layer [Yes, No]
Yes     print_AmaVolWatLay  ! Mass volatilised in water layer [Yes, No]
Yes     print_AmaSedInWatLay ! Mass penetrated into sediment from water layer [Yes, No]
Yes     print_AmaSedOutWatLay ! Mass transferred from sediment into water layer! [Yes, No]
Yes     print_AmaDwnWatLay  ! Mass flowed across downstream boundary out of water layer
Yes     print_AmaUpsWatLay  ! Mass flowed across upstream boundary into water layer
Yes     print_AmaDrfWatLay  ! Mass entered water layer by spray drift [Yes, No]
Yes     print_AmaAtmDepWatLay ! Mass entered water layer by atmospheric deposition [Yes, No]
Yes     print_AmaDraWatLay  ! Mass entered water layer by drainage [Yes, No]
Yes     print_AmaRnoWatLay  ! Mass entered water layer by runoff [Yes, No]
Yes     print_AmaTraSed     ! Mass transformed in sediment layer [Yes, No]
Yes     print_AmaForSed     ! Mass formed in sediment layer [Yes, No]
Yes     print_AmaWatLayInSed ! Mass transferred into water layer from sediment layer
Yes     print_AmaWatLayOutSed ! Mass transferred from water layer into sediment layer [Yes, No]
Yes     print_AmaDwnSed     ! Mass leaving sediment layer across lower boundary [Yes, No]
Yes     print_AmaErsSed     ! Mass entering sediment layer by erosion [Yes, No]
No      print_VolErrWatLay  ! Volume error in waterbody [Yes, No]
No      print_AmaErrWatLay  ! Mass error in mass balance of the waterlayer [Yes, No]

```

Figure 3.8 The Output control section in the TOXSWA input file

3.4 The meteo input file

The meteorological input file contains the average temperatures in the water body system per month. An example of a Name.met file is shown in Figure 3.9.

```
*
* TOXSWA input file
* Filename: C:\SwashProjects\project_H_sw\toxswa\Weiherbach.met
* Weather station: Weiherbach
* Contents: Input data for TOXSWA concerning temperature
* Date : 27-Mar-2013
*
*-----
* temperature in water and sediment per month
1975 1 4.85
1975 2 4.18
1975 3 5.35
.
.
.
1994 10 9.66
1994 11 8.84
1994 12 6.35
! - - o^C : unit
! 0 .... 9999 1 .... 12 4. .... 50 : range
*
*-----END OF FILE-----
```

Figure 3.9 Example of a meteo input file.

Monthly averaged temperatures might be calculated from daily air temperatures in case measured values are not available. TOXSWA calculates transformation and volatilization rates according to water body temperature.

3.5 The drainage and runoff input files

The RunId.m2t file is an output file of the MACRO model containing the hourly water and pesticide fluxes entering the water body by drainage. An example of a RunID.m2t file is shown in Figure 3.10. In the header the dates of the applications and corresponding application rates are indicated. TOXSWA reads the dates of the applications to determine the dates of the spray drift events.

```
* MACRO to TOXSWA input file
(C:\SwashProjects\project_EXSW2\MACRO\cereals_winter\macro00001_p.m2t) created on 24/09/2012
09:33:04
* MACRO in FOCUS Version 4.4.2
* Output File = C:\SwashProjects\project_EXSW2\MACRO\cereals_winter\macro003.bin
* Parameter File = C:\SwashProjects\project_EXSW2\MACRO\cereals_winter\paren003.par
* Run ID = 1
* Compound : EXSW2
* Scenario : D4
* Surface water (drained at 1.2 m depth and 10 m spacing)
*
* Simulation from 19790101 to 19860430, application every year
* (6 year warm-up, outputs for the last 16 months)
*
* Crop : Cereals, winter, not irrigated
*
$ Application type : Ground spray
* Number of applications (-)
# 3
* Application (-) Date (-) Mass (g ai/ha)
# 1 9-Sep-1985 1000
# 2 19-Sep-1985 750
# 3 25-Oct-1985 500
*
*Time (YYYYMMDDHHMM) Drainage mm/h Pest._flux_to_drains_mg/m2/h
198501010030 6.778806E-02 1.866895E-02
198501010130 6.741687E-02 1.854957E-02
198501010230 6.704471E-02 1.842992E-02
198501010330 6.667209E-02 1.831019E-02
198501010430 0.0662996 1.819056E-02
198501010530 6.592772E-02 1.807118E-02
198501010630 6.555685E-02 1.795218E-02
198501010730 6.518733E-02 1.783367E-02
198501010830 6.481946E-02 1.771574E-02
198501010930 6.445357E-02 0.0175985
```

Figure 3.10 The MACRO output file containing hourly water and pesticide fluxes, entering the water body by drainage for TOXSWA.


```
* PRZM3 output file / TOXSWA input file
*
* Filename: C:\SwashProjects\project_H_sw\przm\cereals_winter\00003-C1.P2T
*
* Generated by: TSR FOCUS_PRZM_SW_3.1.1, 12 December 20
* Created: 20130627232606.741
*
* PRZM3 input files
* Chem file: Rl-CW-.INP
* Met file: Rlnoirr.met
*
*
* Chemical: EXSW2
* Crop: Cereals, Winter
* Scenario: Rl
* Description:
*
*
* Selected 50th percentile year: 1978
* Season of first application: autumn (Oct-Feb)
* Selected 12 month period: 01-Oct-1978 to 30-Sep-1979
* Application type: ground spray)
* Number of applications:
# 1
*
* Application Time (YYYYMMDDHHMM) Mass (g ai/ha)
# 01 14-Nov-1978-09:00 1000.0000
*
*
*
*
* Runoff Volume Runoff flux Erosion Mass Erosion Flux
Infiltration
* Time (YYYYMMDDHHMM) (mm/h) (mg as/m2/h) (kg/h) (mg as/m2/h) (mm/h)
01-Oct-1978-01:00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1213E-01
01-Oct-1978-02:00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1213E-01
01-Oct-1978-03:00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1213E-01
01-Oct-1978-04:00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1213E-01
01-Oct-1978-05:00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1213E-01
01-Oct-1978-06:00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1213E-01
01-Oct-1978-07:00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1213E-01
01-Oct-1978-08:00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1213E-01
01-Oct-1978-09:00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1213E-01
01-Oct-1978-10:00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.1213E-01
.
```

```

* -----
* TOXSWA REPORT: Header
* Results from the TOXSWA model (c) Alterra
* FOCUS TOXSWA version : 4
* TOXSWA model version : 3.3.1
* TOXSWA created on : 25-Apr-2013
*
* Working directory : C:\SwashProjects\Project_1\TOXSWA
* Run ID : 1
* Input file generated on : 30-09-2013
* -----
*
* Scenario : D4_Pond
* Meteo Station : Skousbo
* Substance : EXSW2
* Flow Type : Variable
* Water Body Type : D4_POND
* Application Scheme : FOCUS_EXAMPLE
* Simulation Period : 01-Jan-1985 to 30-Apr-1986
* -----
*
* End of TOXSWA REPORT: Header
* -----
*
* TOXSWA REPORT: Substance properties and substance loadings
*
* Summary for the following substances
*
* Substance 1: EXSW2
* Molar mass (g.mol-1) : 300.0
* Saturated vapour pressure (Pa) : 0.100E-06 measured at (C) : 20.0
* Water solubility (mg.L-1) : 0.100E+01 measured at (C) : 20.0
* Half-life in water (d) : 100.00 measured at (C) : 20.0
* Half-life in sediment (d) : 300.00 measured at (C) : 20.0
* Kom susp.solids (coef. for sorption on organic matter) (L.kg-1) : 58.00
* Freundlich exponent (-) : 1.00
* Kom sediment (coef. for sorption on organic matter) (L.kg-1) : 58.00
* Freundlich exponent (-) : 1.00
* Kmp (coef. for sorption on macrophytes-dry weight) (L.kg-1) : 0.00
*
* Summary for the substance loadings
*
* Application pattern and deposition by drift on water surface
* Appl.No Date/Hour Mass (g ai.ha-1) Areic mean deposition (mg.m-2)
* 1 10-Sep-1985-09h00 1000.0000 0.1540
* 2 28-Sep-1985-09h00 750.0000 0.1155
* 3 26-Oct-1985-09h00 500.0000 0.0770
*
* Lateral entry: drainage Simulated by: MACRO
* Soil metabolite: Met1
*
* Fraction metabolite formed in water in upstream catchment: 1.0000
**
*
* Maximum hourly fluxes from lateral entries
* Year Type Water/Substance Flux Date
* 1985 Water 0.3529 mm.m-2.hr-1 06-Dec-1985-04h30
* 1985 Drainage EXSW2 0.1191 mg.m-2.hr-1 07-Dec-1985-08h30
* 1985 Drainage EXSW2 2546865.8 ug.L-1 22-Jun-1985-07h30
* 1986 Water 0.1163 mm.m-2.hr-1 23-Jan-1986-00h30
* 1986 Drainage EXSW2 0.03405 mg.m-2.hr-1 23-Jan-1986-01h30
* 1986 Drainage EXSW2 1061606.2 ug.L-1 23-Jan-1986-20h30
*
* End of TOXSWA REPORT: Substance properties and substance loadings

```

Figure 3.12a The summary output file: substance properties and substance loadings.

Substance properties and substance loadings

The main physico-chemical properties of all simulated substances, i.e. the parent and its metabolites, are repeated. Note that the units of parameters may differ from the units of the parameters in the input files.

The application pattern and deposition by spray drift on the water surface is given. Notice that for FOCUS stream scenarios the drift value given in the RunId.sum file differs from the value of the FOCUS drift calculator. Drift calculated with the FOCUS drift calculator is multiplied by 1.2 for stream runs, because of the assumption that 20% of the upstream catchment is treated (FOCUS, 2001). The kind of lateral entry, i.e. drainage or runoff route into surface water is indicated, the soil metabolites that come along, and - only relevant for streams - the correction factor that is used for the fraction metabolite formed in water in the upstream catchment (see Section 4.4.4). The maximum hourly fluxes and the maximum hourly concentrations in drained water or runoff from the entries are given.

```

* -----
* Table: Water balance of the waterbody
* Key to the table
* -----
* DelSto          Change in volume present in water layer (m3)
* VolPrc          Volume entered in water body by precipitation (m3)
* VolDra          Volume entered in water body by drainage (m3)
* VolRun          Volume entered in water body by runoff (m3)
* VolUps          Volume flowed into water body across upstream boundary (m3)
* VolDwn          Volume flowed out of water body across downstream boundary (m3)
* -----
* Monthly water balance terms (m3) in water system of      30.00 m
* -----
* Year Month Identifier DelSto VolPrc VolDra VolRun VolUps VolDwn
* -----
1985 Jan BalWatLay 0.3600 0.0000 104.8401 0.0000 0.0000 203.4459
1985 Feb BalWatLay 0.0900 0.0000 117.6471 0.0000 0.0000 206.8749
1985 Mar BalWatLay 0.6300 0.0000 95.7012 0.0000 0.0000 193.9126
1985 Apr BalWatLay -0.7200 0.0000 100.1232 0.0000 0.0000 196.5287
1985 May BalWatLay -0.1800 0.0000 46.3919 0.0000 0.0000 145.4630
1985 Jun BalWatLay -0.1800 0.0000 5.6284 0.0000 0.0000 101.4468
1985 Jul BalWatLay 0.0000 0.0000 0.0000 0.0000 0.0000 98.8597
1985 Aug BalWatLay 0.0000 0.0000 0.0000 0.0000 0.0000 98.8597
1985 Sep BalWatLay 0.0000 0.0000 0.0000 0.0000 0.0000 95.6707
1985 Oct BalWatLay 0.2700 0.0000 16.6388 0.0000 0.0000 115.2818
1985 Nov BalWatLay -0.0900 0.0000 21.2917 0.0000 0.0000 117.0190
1985 Dec BalWatLay 1.0800 0.0000 433.4568 0.0000 0.0000 531.1980
1986 Jan BalWatLay -0.1800 0.0000 187.0059 0.0000 0.0000 286.0366
1986 Feb BalWatLay -0.7200 0.0000 74.9097 0.0000 0.0000 164.9884
1986 Mar BalWatLay -0.1800 0.0000 25.7239 0.0000 0.0000 124.7873
1986 Apr BalWatLay 0.0000 0.0000 25.1795 0.0000 0.0000 120.7833
* -----
* Annual water balance terms (m3) in water system of      30.00 m
* -----
* Year Identifier DelSto VolPrc VolDra VolRun VolUps VolDwn
* -----
1985 BalWatLay 1.2600 0.0000 941.7191 0.0000 1163.9850 2104.5609
1986 BalWatLay -1.0800 0.0000 312.8190 0.0000 382.6800 696.5956
* -----

```

Figure 3.12b The summary output file: water balance.

Water balance

The elements of the water balance are given in a table with monthly values and in a table with annual values (see Fig. 3.12b). The water balance elements of the water body are also given per month. Note that when only part of the year is simulated, the yearly balance only considers this part of the year.

Mass balance water layer

The mass balance of the substance in the water body is given in tables per month and per year (see Fig. 3.12c). These tables are given for each substance, i.e. the parent and its metabolites. The tables show the numbers with a limited number of decimals for the best readability. Positive values indicate that mass is added, and negative values indicate that mass is reduced.

Mass balance sediment layer

The mass of the sediment in the whole thickness of the sediment of the entire water body is given in tables per month and per year (see Fig. 3.12d). These tables are given for each substance, i.e. the parent and its metabolites.

* Table: Mass balance of substance in the water system of 30.00 m														
* Key to the table														
* -----														
* DelAma	Change in mass present in water layer system (g)													
* AmaIni	Mass initially present in water layer (g)													
* AmaDrf	Loading of water body by drift (g)													
* AmaAtmDep	Loading of water body by atmospheric deposition (g)													
* AmaDra	Loading of water body by drainage (g)													
* AmaRnO	Loading of water body by run-off (g)													
* AmaSedIn	Mass penetrated into sediment (g)													
* AmaSedOut	Mass transferred out of sediment (g)													
* AmaDwn	Mass flowed across downstream boundary end (g)													
* AmaUps	Mass flowed across upstream boundary end (g)													
* AmaTra	Mass transformed in water layer (g)													
* AmaFor	Mass formed in water layer (g)													
* AmaVol	Mass volatilised from water layer (g)													
* -----														
* -----														
* Monthly mass balance terms (g) in water system of 30.00 m for compound: EXSW2														
* Year	Month	DelAma	AmaIni	AmaDrf	AmaAtmDep	AmaDra	AmaRnO	AmaSedIn	AmaSedOut	AmaDwn	AmaUps	AmaTra	AmaFor	AmaVol
* -----														
1985	Jan	14.2506	0.0000	0.0000	0.0000	17.5742	0.0000	-0.6475	0.0000	-2.1935	0.0000	-0.4825	0.0000	-0.0001
1985	Feb	14.1800	14.2506	0.0000	0.0000	21.6214	0.0000	-0.9509	0.0000	-5.4715	0.0000	-1.0186	0.0000	-0.0003
1985	Mar	6.3635	28.4306	0.0000	0.0000	15.0358	0.0000	-0.7980	0.0000	-6.5057	0.0000	-1.3682	0.0000	-0.0004
1985	Apr	6.1106	34.7941	0.0000	0.0000	17.6650	0.0000	-1.0064	0.0000	-8.6359	0.0000	-1.9116	0.0000	-0.0006
1985	May	-4.2694	40.9047	0.0000	0.0000	6.0955	0.0000	-0.5864	0.0000	-6.3179	0.0000	-3.4595	0.0000	-0.0011
1985	Jun	-7.3668	36.6354	0.0000	0.0000	0.5926	0.0000	-0.2271	0.0000	-3.7168	0.0000	-4.0142	0.0000	-0.0013
1985	Jul	-6.9310	29.2685	0.0000	0.0000	0.0000	0.0000	-0.0352	0.0037	-2.8127	0.0000	-4.0854	0.0000	-0.0013
1985	Aug	-5.0770	22.3375	0.0000	0.0000	0.0000	0.0000	0.0000	0.0544	-2.1597	0.0000	-2.9708	0.0000	-0.0009
1985	Sep	-2.9913	17.2605	0.2426	0.0000	0.0000	0.0000	-0.0001	0.0686	-1.6665	0.0000	-1.6354	0.0000	-0.0005
1985	Oct	-0.7788	14.2692	0.0693	0.0000	1.9582	0.0000	-0.0080	0.0431	-1.7146	0.0000	-1.1266	0.0000	-0.0004
1985	Nov	0.0106	13.4904	0.0000	0.0000	2.4736	0.0000	-0.0414	0.0000	-1.7577	0.0000	-0.6637	0.0000	-0.0002
1985	Dec	88.2575	13.5009	0.0000	0.0000	133.6737	0.0000	-3.6698	0.0000	-38.5333	0.0000	-3.2120	0.0000	-0.0010
1986	Jan	7.1366	101.7585	0.0000	0.0000	46.9725	0.0000	-2.6139	0.0000	-32.5532	0.0000	-4.6673	0.0000	-0.0015
1986	Feb	-10.3242	108.8951	0.0000	0.0000	14.7608	0.0000	-1.5517	0.0000	-19.2222	0.0000	-4.3098	0.0000	-0.0013
1986	Mar	-13.8893	98.5708	0.0000	0.0000	3.8465	0.0000	-0.8467	0.0000	-12.7059	0.0000	-4.1819	0.0000	-0.0013
1986	Apr	-11.1214	84.6816	0.0000	0.0000	3.7314	0.0000	-0.4237	0.0000	-10.5778	0.0000	-3.8501	0.0000	-0.0012
* -----														
* -----														
* Annual mass balance terms (g) in water system of 30.00 m for compound: EXSW2														
* Year	DelAma	AmaIni	AmaDrf	AmaAtmDep	AmaDra	AmaRnO	AmaSedIn	AmaSedOut	AmaDwn	AmaUps	AmaTra	AmaFor	AmaVol	
* -----														
1985	101.7585	0.0000	0.3119	0.0000	216.6899	0.0000	-7.9707	0.1698	-81.4857	0.0000	-25.9484	0.0000	-0.0081	
1986	-28.1983	101.7585	0.0000	0.0000	69.3112	0.0000	-5.4360	0.0000	-75.0590	0.0000	-17.0092	0.0000	-0.0053	
* -----														
* -----														

Figure 3.12c The summary output file: mass balance of water layer

```

* Table: Mass balance of substance in the sediment system of      30.00 m
* Key to the table
* -----
* DelAmaSed      Change in mass present in sediment system (g)
* AmaIniSed      Mass initially present in sediment (g)
* AmaErs         Loading of sediment by erosion (g)
* AmaWaterIn     Mass transfered to water layer (g)
* AmaWaterOut    Mass transfered from water layer (g)
* AmaDwnSed      Mass flowed across boundary to deeper layers (g)
* AmaTraSed      Mass transformed in sediment (g)
* AmaFor         Mass formed in sediment (g)
* -----
*
* -----
* Monthly mass balance terms (g) in sediment of waterbody system of      30.00 m for compound:  EXSW2
* Year  Month  DelAmaSed  AmaIniSed  AmaErs  AmaWatIn  AmaWatOut  AmaDwnSed  AmaTra  AmaFor
* -----
1985   Jan    0.6424    0.0000    0.0000    0.0000    0.6475    0.0000    -0.0051    0.0000
1985   Feb    0.9354    0.6424    0.0000    0.0000    0.9509    0.0000    -0.0155    0.0000
1985   Mar    0.7684    1.5777    0.0000    0.0000    0.7980    0.0000    -0.0295    0.0000
1985   Apr    0.9606    2.3462    0.0000    0.0000    1.0064    0.0000    -0.0458    0.0000
1985   May    0.4807    3.3068    0.0000    0.0000    0.5864    0.0000    -0.1056    0.0000
1985   Jun    0.0707    3.7875    0.0000    0.0000    0.2271    0.0000    -0.1564    0.0000
1985   Jul   -0.1694    3.8582    0.0000   -0.0037    0.0352    0.0000    -0.2010    0.0000
1985   Aug   -0.2343    3.6888    0.0000   -0.0544    0.0000    0.0000    -0.1799    0.0000
1985   Sep   -0.1852    3.4545    0.0000   -0.0686    0.0001    0.0000    -0.1167    0.0000
1985   Oct   -0.1245    3.2693    0.0000   -0.0431    0.0080    0.0000    -0.0893    0.0000
1985   Nov   -0.0099    3.1449    0.0000    0.0000    0.0414    0.0000    -0.0513    0.0000
1985   Dec    3.5949    3.1350    0.0000    0.0000    3.6698    0.0000    -0.0750    0.0000
1986   Jan    2.4921    6.7298    0.0000    0.0000    2.6139    0.0000    -0.1218    0.0000
1986   Feb    1.4139    9.2219    0.0000    0.0000    1.5517    0.0000    -0.1378    0.0000
1986   Mar    0.6788   10.6358    0.0000    0.0000    0.8467    0.0000    -0.1679    0.0000
1986   Apr    0.2374   11.3145    0.0000    0.0000    0.4237    0.0000    -0.1862    0.0000
* -----
*
* -----
* Annual mass balance terms (g) in sediment system of      30.00 m for compound:  EXSW2
* Year      DelAmaSed  AmaIniSed  AmaErs  AmaWatIn  AmaWatOut  AmaDwnSed  AmaTraSed  AmaForSed
* -----
1985      0.0000    0.0000    0.0000   -0.1698    7.9707    0.0000    -1.0712    0.0000
1986      0.0000    0.0000    0.0000    0.0000    5.4360    0.0000    -0.6138    0.0000
* -----

```

Figure 3.12d The summary output file: mass balance of sediment system

```

* -----
* TOXSWA REPORT: Exposure in Waterbody

* Table: Annual maximum exposure concentrations in water layer of substance: EXSW2
* In segment from 0.00 to 30.00 m in water body
* -----
* Year                Concentration          Date                Daynr
*                   µg.L-1
* -----
1985                  112.8        31-Dec-1985-23h00        365
1986                  120.7        01-Feb-1986-16h00        397

* Tables: Maximum exposure concentrations in water layer
* In segment from 0.00 to 30.00 m in water body
* Actual concentrations PECsw as well as PECsed refer to momentary concentrations
* occurring 1, 2 etc days after the global maximum concentration.
* The Time Weighted Average Exposure Concentrations (TWAEC) have been calculated
* for a moving time frame and have been allocated to the last day of the period considered

* Table: PEC in water layer of substance: EXSW2
* -----
*                   Concentration          Date                Daynr
*                   µg.L-1
* -----
Global max            120.7        01-Feb-1986-16h00        397
(incl. suspend.solid  120.7        01-Feb-1986-16h00        397)
PECsw_1_day           120.6        02-Feb-1986-16h00        398
PECsw_2_days          120.5        03-Feb-1986-16h00        399
PECsw_4_days          120.0        05-Feb-1986-16h00        401
PECsw_7_days          119.0        08-Feb-1986-16h00        404
PECsw_14_days         115.9        15-Feb-1986-16h00        411
PECsw_21_days         112.5        22-Feb-1986-16h00        418
PECsw_28_days         109.0        01-Mar-1986-16h00        425
PECsw_42_days         101.9        15-Mar-1986-16h00        439
PECsw_50_days         97.93        23-Mar-1986-16h00        447
PECsw_100_days        -            -            -
* -----
* Legend: - in table means PECsw is later than end of simulated period: 30-Apr-1986

* Table: Maximum Time Weighted Averaged Exposure Concentrations substance: EXSW2
* -----
*                   Concentration          Date                Daynr
*                   µg.L-1
* -----
TWAECsw_1_day         120.7        01-Feb-1986-23h00        397
TWAECsw_2_days        120.7        02-Feb-1986-12h00        398
TWAECsw_4_days        120.6        03-Feb-1986-13h00        399
TWAECsw_7_days        120.5        05-Feb-1986-06h00        401
TWAECsw_14_days       119.9        09-Feb-1986-19h00        405
TWAECsw_21_days       119.1        14-Feb-1986-23h00        410
TWAECsw_28_days       118.1        20-Feb-1986-09h00        416
TWAECsw_42_days       115.7        01-Mar-1986-22h00        425
TWAECsw_50_days       115.1        21-Feb-1986-14h00        417
TWAECsw_100_days      109.9        30-Mar-1986-14h00        454
* -----

```

Figure 3.12e The summary output file: exposure concentrations in water.

Exposure concentrations in water

First a table with the maximum Predicted Environmental Concentrations (PEC) in the last segment downstream in the water body for each simulated year is given. If TOXSWA is used for simulation of periods that extend the standard FOCUS period (16 months for drainage runs, 12 months for runoff runs), the concentrations in this table can be used to select a selected percentile concentration of the annual maximum concentrations.

The next table gives the maximum Predicted Environmental Concentration (PEC) in the last segment downstream in the water body, followed by the PEC at selected time intervals after the occurrence of the maximum concentration. Apart from the global maximum concentration also the total concentration is given, i.e. mass dissolved and mass adsorbed to suspended solids. For substances with high sorption coefficients the total concentration is higher than the concentration dissolved.

In the last table the Time Weighted Average Exposure Concentrations (TWAECs) in the last segment downstream in the water body are given. These concentrations are used in the risk assessment to evaluate chronic exposure.

```

* Tables: Maximum exposure content in sediment
-----
* In the top      5.00 cm sediment located under
* the water body segment from      0.00 to      30.00m,
* the content is expressed as µg substance per kg dry sediment.

* Table: PEC in sediment of substance: EXSW2
* -----
*                               Content          Date          Daynr
*                               µg.kg-1
* -----
Global max                     283.1      14-Apr-1986-13h00      469
PECsed_1_day                   283.1      15-Apr-1986-13h00      470
PECsed_2_days                  283.1      16-Apr-1986-13h00      471
PECsed_4_days                  283.0      18-Apr-1986-13h00      473
PECsed_7_days                  282.9      21-Apr-1986-13h00      476
PECsed_14_days                 282.2      28-Apr-1986-13h00      483
PECsed_21_days                 -              -              -
PECsed_28_days                 -              -              -
PECsed_42_days                 -              -              -
PECsed_50_days                 -              -              -
PECsed_100_days                -              -              -
* -----
* Legend: - in table means PECsed is later than end of simulated period:  30-Apr-1986

* Table: Maximum Time Weighted Averaged Exposure Content substance: EXSW2
* -----
*                               Content          Date          Daynr
*                               µg.kg-1
* -----
TWAECsed_1_day                 283.1      15-Apr-1986-01h00      470
TWAECsed_2_days                283.1      15-Apr-1986-13h00      470
TWAECsed_4_days                283.1      16-Apr-1986-13h00      471
TWAECsed_7_days                283.1      18-Apr-1986-00h00      473
TWAECsed_14_days               283.0      21-Apr-1986-10h00      476
TWAECsed_21_days               282.9      24-Apr-1986-21h00      479
TWAECsed_28_days               282.8      28-Apr-1986-13h00      483
TWAECsed_42_days               282.2      01-May-1986-00h00      486
TWAECsed_50_days               281.5      01-May-1986-00h00      486
TWAECsed_100_days              266.1      01-May-1986-00h00      486
* -----

* End of TOXSWA REPORT: Exposure in Waterbody
* -----

* The run time was      0 minutes and 39 seconds

```

Figure 3.12f The summary output file: exposure concentrations in sediment.

Exposure concentrations in sediment

The first table presents the maximum content of the substance in the top layer of the sediment below the last segment downstream in the water body. The maximum content is followed by the contents at selected time intervals after the occurrence of the maximum content. The thickness of the top layer of the sediment is indicated in the header of the table and is set via input parameter `ThiLayTgt` (see Section 3.3.11). The default value for FOCUS scenarios is 5 cm.

The second table presents the Time Weighted Average Exposure content in the top layer of the sediment below the last segment downstream in the water body. These concentrations are used in the risk assessment to evaluate chronic exposure.

3.7 The comprehensive output file

The comprehensive output file (`runID.out`) presents extensive output of the TOXSWA simulation based on the settings in the Output control section of the TOXSWA input file (see 3.3.11). A technical description of the output in the file is given in Annex 3.

As described in Section 3.3.11, the output is rather flexible. The print interval can be set (record `DelTimPrn`), a format for the date can be set (record `DateFormat`), output distances can be specified (table `OutputDistances`), output depths can be specified (table `OutputDepths`), and for each variable in the output list, a print flag can be set indicating whether the variable is to be printed (record `print_`).

Two types of output are written to the comprehensive output file:

- Output as a function of time. This type of output is produced at regular intervals. This interval is controlled by the variable `DelTimPrn`.
- Output as function of distance in the water layer and as a function of depth in the sediment layer. This type of model output is produced only at the dates specified in the `HorizontalProfiles` table.

All types of model output are written in records.

3.7.1 Output as a function of time

Time dependent model outputs are written in records with the following general format:

```
Time      Date      Identifier  Value(1)  ....  Value(n)
```

where n is:

- one in the case of ordinary (distance and depth independent) variables,
- the number of distances specified in the `OutputDistances` table

For variables in sediment that are a function of depth n records are written to the output file, with the following general format.

```
Time      Date      Identifier  Node(n)  Value(1)  ....  Value(m)
Time      Date      Identifier  Node(n)  Value(1)  ....  Value(m)
```

where m is the number of depths specified in the `OutputDepths` table.

The box below shows a part of the output file, which was produced with the following control settings:

1. `DateFormat` was set at `DaysFromSta`.
2. `RealFormat` was set at `e14.6`
3. `OutputDistances` was set at 3, 50 and 98 m. These distances are in the 0-5 m, 45-50 m and 95-100 m segment with nodal points situated at 2.5, 47.5, and 97.5 m distance in the watercourse in segment numbers 1, 10 and 20. The distances of the nodal points are listed in the second record directly after the header, with label 'x'.
4. Output was requested for the variables `DepWat`, `ConLiqWatLay`, `ConLiqWatLayCur`, `ConSysSed`, `AmaErrWatLay`.
5. The name of the substance is coupled as label to the output variable, when the output variable is for a substance. In the example 'EXSW3' in `ConLiqWatLay_EXSW3`.
6. In the records showing a variable that has distance, as fourth label the segment number is indicated. In the example `ConSysSed_EXSW3` is shown for segment 1, 10 and 20.

```
* -----
* Results from the TOXSWA model (c) Alterra
* FOCUS TOXSWA version : 4
* TOXSWA model version : 3.3.2
* TOXSWA created on : 12-Sep-2013
*
* Working directory : C:\SWASHprojects\Project_EXSW3\toxswa
* Run ID : 3
* Input file generated on : 09-05-2012
* -----
*
* 0.000 Z 0.500000E-03 0.850000E-01
* 0.000 X 0.250000E+01 0.475000E+02 0.975000E+02
* Option PrintCumulatives was set to false
* Unit for DepWat is (m)
* Unit for ConLiqWatLay is (g.m-3)
* Unit for ConLiqWatLayCur is (g.m-3)
* Unit for ConSysSed is (g.m-3)
* Unit for AmaErrWatLay is (g)
*
*
* 62.063 02-Dec-1978-01h30 DepWat 0.428900E+00 0.428900E+00 0.428900E+00
* 62.063 02-Dec-1978-01h30 ConLiqWatLay_EXSW3 0.253926E-07 0.160128E-06 0.325708E-06
* 62.083 02-Dec-1978-02h00 ConLiqWatLayCur_EXSW3 0.252750E-07 0.159384E-06 0.324187E-06
* 62.063 02-Dec-1978-01h30 ConSysSed_EXSW3 1 0.144383E-03 0.770485E-10
* 62.063 02-Dec-1978-01h30 ConSysSed_EXSW3 10 0.183005E-03 0.329764E-09
* 62.063 02-Dec-1978-01h30 ConSysSed_EXSW3 20 0.222603E-03 0.575947E-09
* 62.063 02-Dec-1978-01h30 AmaErrWatLay_EXSW3 0.184436E-12
```

Figure 3.13 The comprehensive output file; the header and an excerpt of the hourly output.

3.7.2 Horizontal and vertical profiles of some selected variables

Horizontal profiles in the water layer and vertical profiles in the sediment layer are produced only at times specified in the `HorizontalProfiles` table. For each requested time and for each substance, a series of records is produced with the name `XProfile_subst` or `ZProfile_subst` (where `subst` must be substituted by the appropriate substance name). The records in the output give the following variables (see below):

```
61.979 01-Dec-1978 XProfile_EXSW3 0 .250000E+01 0.428900E+00 0.510000E+01 0.257659E-07
61.979 01-Dec-1978 XProfile_EXSW3 0. 750000E+01 0.428900E+00 0.510000E+01 0.394394E-07
61.979 01-Dec-1978 XProfile_EXSW3 0. 125000E+02 0.428900E+00 0.510000E+01 0.534988E-07
61.979 01-Dec-1978 XProfile_EXSW3 0. 175000E+02 0.428900E+00 0.510000E+01 0.679388E-07
61.979 01-Dec-1978 XProfile_EXSW3 0. 225000E+02 0.428900E+00 0.510000E+01 0.827586E-07
61.979 01-Dec-1978 XProfile_EXSW3 0. 275000E+02 0.428900E+00 0.510000E+01 0.979488E-07
61.979 01-Dec-1978 XProfile_EXSW3 0. 325000E+02 0.428900E+00 0.510000E+01 0.113515E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 375000E+02 0.428900E+00 0.510000E+01 0.129461E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 425000E+02 0.428900E+00 0.510000E+01 0.145786E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 475000E+02 0.428900E+00 0.510000E+01 0.162492E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 525000E+02 0.428900E+00 0.510000E+01 0.179576E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 575000E+02 0.428900E+00 0.510000E+01 0.197031E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 625000E+02 0.428900E+00 0.510000E+01 0.214837E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 675000E+02 0.428900E+00 0.510000E+01 0.232956E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 725000E+02 0.428900E+00 0.510000E+01 0.251311E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 775000E+02 0.428900E+00 0.510000E+01 0.269743E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 825000E+02 0.428900E+00 0.510000E+01 0.287931E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 875000E+02 0.428900E+00 0.510000E+01 0.305224E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 925000E+02 0.428900E+00 0.510000E+01 0.320312E-06
61.979 01-Dec-1978 XProfile_EXSW3 0. 975000E+02 0.428900E+00 0.510000E+01 0.330538E-06
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.500000E-03 0.600000E+00 0.146501E-03 0.436515E-04
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.150000E-02 0.600000E+00 0.431128E-03 0.128459E-03
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.250000E-02 0.600000E+00 0.694070E-03 0.206805E-03
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.350000E-02 0.600000E+00 0.923499E-03 0.275165E-03
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.500000E-02 0.600000E+00 0.120337E-02 0.358554E-03
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.700000E-02 0.600000E+00 0.136766E-02 0.407508E-03
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.900000E-02 0.600000E+00 0.132956E-02 0.396155E-03
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.125000E-01 0.600000E+00 0.100129E-02 0.298345E-03
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.175000E-01 0.600000E+00 0.432430E-03 0.128847E-03
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.250000E-01 0.600000E+00 0.591184E-04 0.176149E-04
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.350000E-01 0.600000E+00 0.447065E-05 0.133207E-05
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.450000E-01 0.600000E+00 0.291278E-06 0.867890E-07
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.600000E-01 0.600000E+00 0.678932E-08 0.202294E-08
61.979 01-Dec-1978 ZProfile_EXSW3 1 -0.850000E-01 0.600000E+00 0.745480E-10 0.22123E-10
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.500000E-03 0.600000E+00 0.185703E-03 0.553319E-04
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.150000E-02 0.600000E+00 0.545579E-03 0.162561E-03
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.250000E-02 0.600000E+00 0.877896E-03 0.261577E-03
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.350000E-02 0.600000E+00 0.116765E-02 0.347912E-03
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.500000E-02 0.600000E+00 0.152072E-02 0.453112E-03
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.700000E-02 0.600000E+00 0.172678E-02 0.514510E-03
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.900000E-02 0.600000E+00 0.167694E-02 0.499659E-03
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.125000E-01 0.600000E+00 0.126002E-02 0.375434E-03
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.175000E-01 0.600000E+00 0.545426E-03 0.162515E-03
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.250000E-01 0.600000E+00 0.775462E-04 0.231056E-04
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.350000E-01 0.600000E+00 0.670304E-05 0.199724E-05
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.450000E-01 0.600000E+00 0.588053E-06 0.175216E-06
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.600000E-01 0.600000E+00 0.211599E-07 0.630479E-08
61.979 01-Dec-1978 ZProfile_EXSW3 10 -0.850000E-01 0.600000E+00 0.322112E-09 0.959764E-10
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.500000E-03 0.600000E+00 0.225902E-03 0.673096E-04
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.150000E-02 0.600000E+00 0.662732E-03 0.197467E-03
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.250000E-02 0.600000E+00 0.106591E-02 0.317600E-03
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.350000E-02 0.600000E+00 0.141717E-02 0.422259E-03
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.500000E-02 0.600000E+00 0.184462E-02 0.549622E-03
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.700000E-02 0.600000E+00 0.209230E-02 0.623421E-03
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.900000E-02 0.600000E+00 0.202917E-02 0.604610E-03
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.125000E-01 0.600000E+00 0.151965E-02 0.452794E-03
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.175000E-01 0.600000E+00 0.657316E-03 0.195854E-03
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.250000E-01 0.600000E+00 0.955653E-04 0.284746E-04
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.350000E-01 0.600000E+00 0.888203E-05 0.264649E-05
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.450000E-01 0.600000E+00 0.878439E-06 0.261739E-06
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.600000E-01 0.600000E+00 0.352111E-07 0.104915E-07
61.979 01-Dec-1978 ZProfile_EXSW3 20 -0.850000E-01 0.600000E+00 0.563257E-09 0.167828E-09
```

Figure 3.14 The comprehensive output file; an excerpt of the profile output.

Horizontal profile for the water layer

1. Day number from start of simulation
2. Date and time
3. Xprofile label indicating horizontal profile in water layer
4. Distance middle of segment from start of water body (m)
5. Water depth (m)
6. Temperature (°C)
7. Dissolved concentration in water (g m^{-3})

Vertical profile for the sediment layer

1. Day number from start of simulation
2. Date and time
3. Zprofile label indicating vertical profile in sediment layer
4. Segment number in water layer, below which vertical profile in sediment is given
5. Depth middle of segment (m)
6. Pore fraction, ($\text{m}^3 \text{m}^{-3}$)
7. Total concentration in the sediment system (g m^{-3})
8. Dissolved concentration in the sediment system (g m^{-3})

3.8 The intermediate output files

For a simulation run TOXSWA firstly simulates the hydrology of the water body, secondly sets the temperature for the water body, and finally simulates the fate of the pesticide in the water body. The simulation of the hydrology results in an intermediate output file runID.hyd. The monthly temperatures are read from the meteo input file and subsequently translated to temperatures for each hour in the runID.met file. The intermediate output files runID.hyd and runID.met are used as input for the pesticide fate simulation.

The intermediate hydrology file contains the discharge(s) and water depth of the water body for each hour. An example of the runID.hyd file is shown in Figure 3.15. Time dependent model outputs are written in records with the following format:

```
Time   Date   Value[Discharge] (1) .... Value[Discharge] (n)   Value[WaterDepth]
```

where n is the number of segments in the water body + 1. The discharge across the boundaries of the segments is given. Hence for the pond, consisting of one segment, i.e. $n = 2$, the discharge across the upstream boundary of the segment and the discharge across the downstream boundary of the single segment is given. For the water depth a single value is given at the end of the record.

* Time	Date	Qbou (0) ($\text{m}^3 \cdot \text{s}^{-1}$)	QBou (1) ($\text{m}^3 \cdot \text{s}^{-1}$)	DepWat (m)
* 0.000	01-Jan-1985	0.3691E-04	0.3691E-04	1.0012
0.042	01-Jan-1985-01h00	0.1278E-03	0.5298E-04	1.0016
0.083	01-Jan-1985-02h00	0.1278E-03	0.6745E-04	1.0018
0.125	01-Jan-1985-03h00	0.1277E-03	0.7985E-04	1.0021
0.167	01-Jan-1985-04h00	0.1276E-03	0.9011E-04	1.0022
0.208	01-Jan-1985-05h00	0.1274E-03	0.9839E-04	1.0024
0.250	01-Jan-1985-06h00	0.1271E-03	0.1049E-03	1.0025

Figure 3.15 The intermediate output file runID.hyd of a pond location.

The intermediate temperature file gives the temperature of the water body for each hour. An example of the runID.met file is shown in Figure 3.16. Time dependent model outputs are written in records with the following format:

```
Time   Date   Value
```

where in the third column the value of the temperature is given in Kelvin.

* Time	Date	TemWat (K)
* 0.042	01-Jan-1985-01h00	277.1500
0.083	01-Jan-1985-02h00	277.1500
0.125	01-Jan-1985-03h00	277.1500
0.167	01-Jan-1985-04h00	277.1500
0.208	01-Jan-1985-05h00	277.1500
0.250	01-Jan-1985-06h00	277.1500

Figure 3.16 The intermediate output file runID.tem.

4 User's guide for the TOXSWA user interface

4.1 Introduction

This chapter gives an overview of the TOXSWA Graphical User Interface (GUI), which is an integrated environment for data storage and data retrieval, model control and viewing the output data (Figure 4.1).

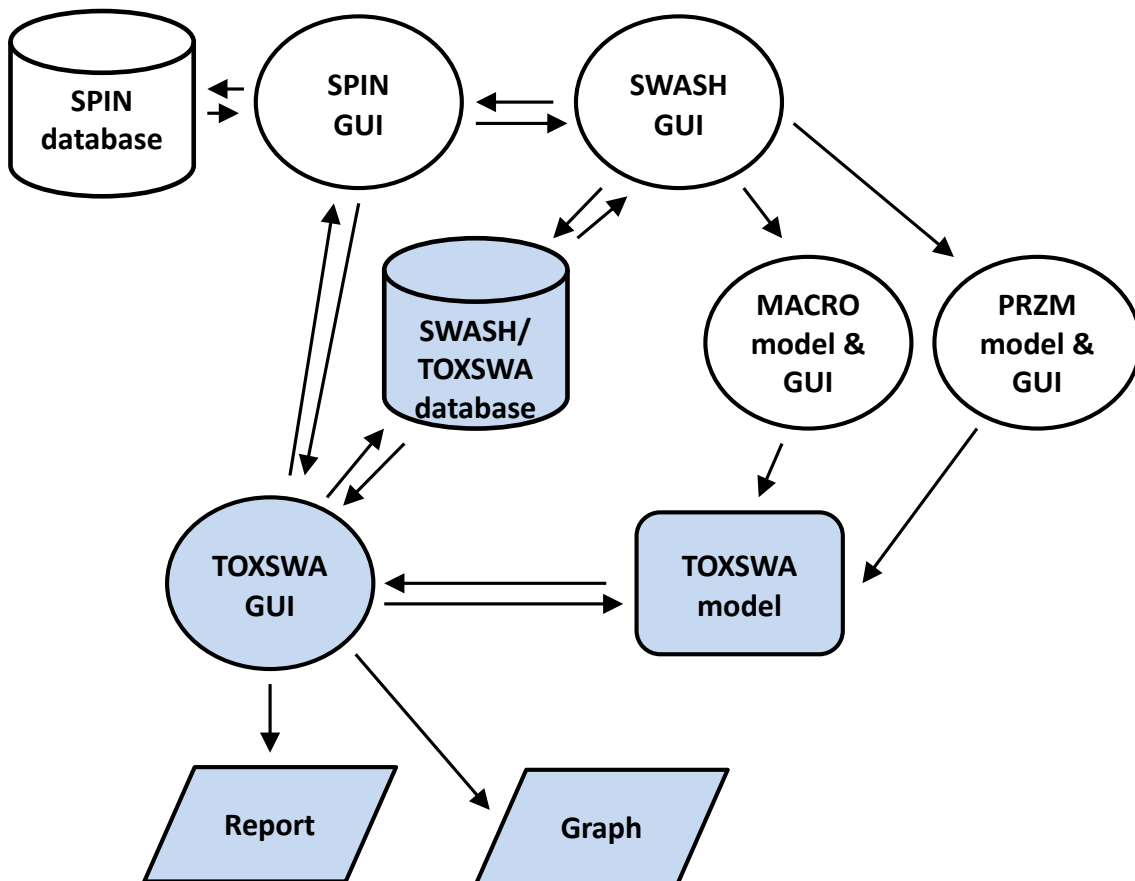


Figure 4.1 Overview of the TOXSWA modelling system (in blue) and its relations with SWASH, SPIN, and the MACRO and PRZM models.

The TOXSWA GUI is linked to the relational databases of SWASH/TOXSWA and SPIN for easy data access. The GUI generates the input files for the TOXSWA model and calls the model. To be able to run TOXSWA (in its transient flow mode; see 3.3.6) the model needs input from either the MACRO model or the PRZM model. The SWASH GUI helps the user to compose consistent runs for this sequence of models. The summary output of TOXSWA can be viewed via the TOXSWA GUI. More comprehensive outputs ('Reports') can be viewed with the Graphical User Interface as well.

This modelling system obviously is quite complex. With the TOXSWA Graphical User Interface, you do not need to bother about all the relationships. The TOXSWA Graphical User Interface makes it easy to:

- access standard scenarios as defined by the FOCUS Surface Water Scenarios Working Group (FOCUS, 2001);
- select one or more model runs for execution;
- actually perform one or several model runs;

- display a summary report containing annual water and mass balances, the maximum concentration in surface water and sediment of the water body, and the output as agreed in the FOCUS Surface Water Scenarios Working Group (FOCUS, 2001);
- display model results graphically;
- export graphs in several formats (bitmap, metafile, PDF, postscript, JPEG, GIF, PCX).

Section 4.2 describes shortly the installation of the FOCUS_TOXSWA software. Section 4.3 describes how FOCUS Step 3 runs can be executed with the TOXSWA GUI. In Sections 4.4 – 4.11 the set-up of the TOXSWA GUI is described in full detail, to enable the user to perform FOCUS Step 4 and other runs. Section 4.12 describes the graphical output that can be viewed.

The SWASH/TOXSWA database and SWASH GUI are designed to facilitate the set-up of FOCUS Step 3 runs. The SWASH/TOXSWA database contains data for the FOCUS drift calculator, the drainage model FOCUS_MACRO, the runoff model FOCUS_PRZM_SW and for TOXSWA. The SWASH GUI is used to set up the input for SPIN, FOCUS drift calculator, MACRO, PRZM and TOXSWA. How to create, edit and manage substances in SPIN is described by Van Kraalingen *et al.* (2013).

Figure 4.2 shows the hierarchy within the TOXSWA GUI. The highest level of the TOXSWA GUI (level 1) is the project level. This level is performed in SWASH for FOCUS Step 3 projects and it is performed in the TOXSWA GUI for FOCUS Step 4 and other projects.

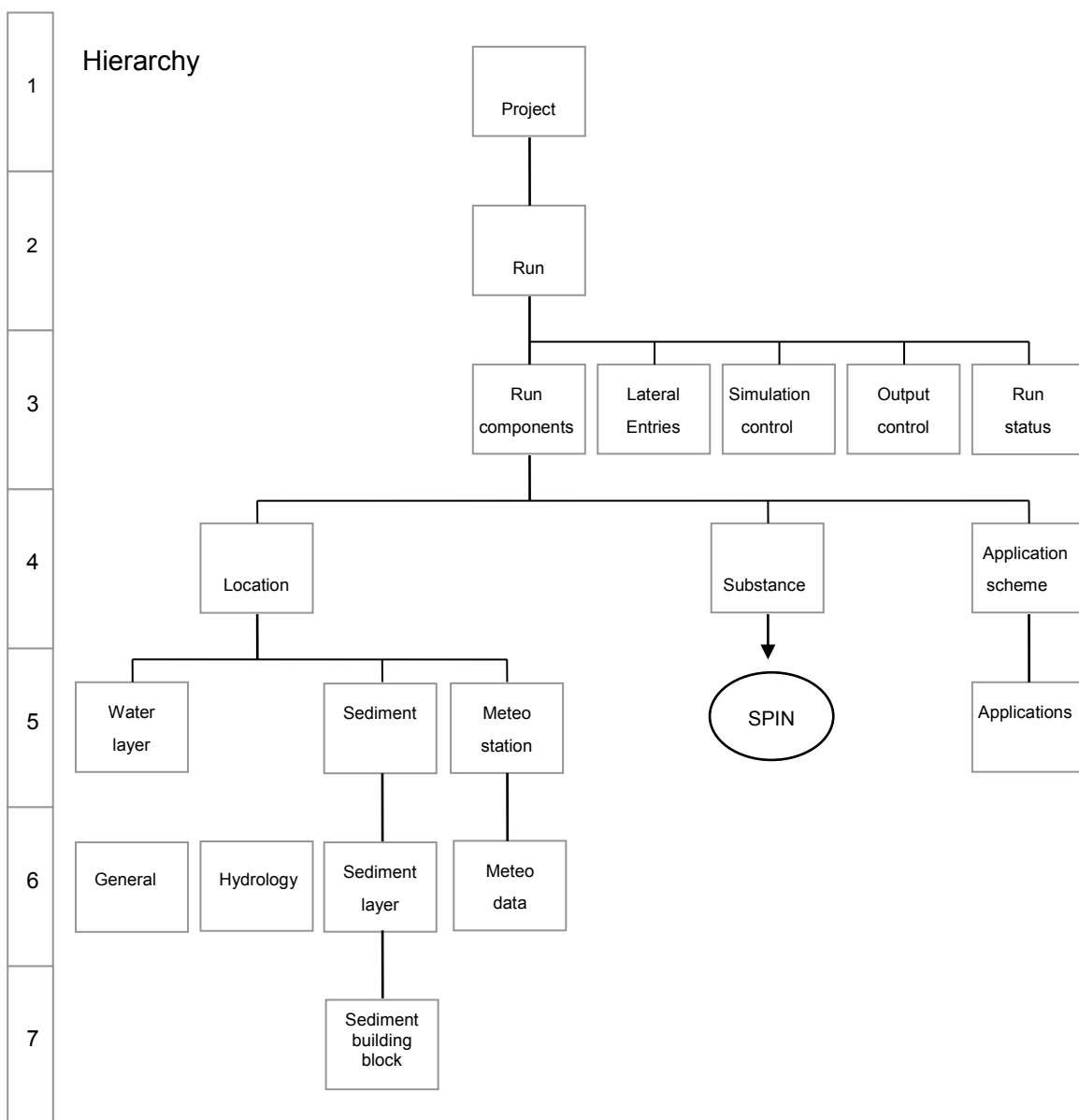


Figure 4.2 Hierarchies within the TOXSWA GUI.

The second level is the model-run level. At the third level, the Run components combine a location scenario, a substance and an application scheme. The Lateral entries contain data concerning the type of lateral entries (drainage or runoff) and the path to the *.m2t or *.p2t file. The Simulation and Output control entries give access to parameters like the start and end time of the simulation, and output control data. Also part of level 3 is the Run status, which gives information about run ID, creation date and modification date of the run. After completion of a run, the performance of the run is listed in the run status.

A run is composed of a location, a substance and an application scheme (level 4). At level 5 to 7 these three run components are further defined. The left-hand side levels 5 to 7 in the diagram show the building blocks of the FOCUS scenarios. A scenario is defined by its water layer, sediment, meteo station and hydrology. The hydrology data are subdivided in data defining the individual water body characteristics like bottom slope, distance to weir (level 5). For watercourses, data for the representative channel are given at level 6 (Hydrology). The entire sediment layer is subdivided into sediment sub layers (level 6). The sediment sub layers are defined by a specific sediment building block (level 7). The meteo station contains the meteo data (level 6).

The substance entry at level 4 gives the name of the substance, which can be a parent or a metabolite. The properties of the substance are entered via the SPIN GUI into the SPIN database, i.e. the general physico-chemical properties, the sorption parameters and the transformation rates in water and in sediment.

At level 4, the application scheme is pesticide and scenario dependent. At level 5, the application rate and spray drift deposition are entered in the spray drift events section.

4.2 Getting Started

After installing SPIN and SWASH, the TOXSWA software package can be installed. When FOCUS_TOXSWA has been installed, the TOXSWA GUI can be started directly via the start menu or via a shortcut on the desktop (if you copied the shortcut of the TOXSWA GUI to your desktop during installation of FOCUS_TOXSWA). The TOXSWA GUI can also be started indirectly via the TOXSWA button in SWASH. Please note that it is not possible to have both software shells, SWASH and TOXSWA, running at the same time on your PC, because they use the same SWASH/TOXSWA database.

4.3 Generating FOCUS Step 3 runs

TOXSWA supports scenario calculations set up by the FQrum for the Co-ordination of pesticide fate models and their Use, FOCUS. Generating FOCUS projects and runs can only be done in SWASH (Fait *et al.*, 2013). SWASH only prepares standard Step 3 FOCUS runs. These can be executed via the TOXSWA GUI. The pesticide is entered and stored in SPIN. In FOCUS Step 3 runs, all selections and parameters have been locked, except some options for output. For the preparation of FOCUS Step 4 runs with TOXSWA, a FOCUS Step 3 project prepared by SWASH can be copied in the TOXSWA GUI. Then it becomes a FOCUS Step 4 project and some of the input values can be changed.

4.4 Preparations

FOCUS runs are organized in so-called projects: specific combinations of a substance, a crop and an application scheme. Therefore, a project contains a series of runs that need to be done to obtain exposure concentrations in the relevant FOCUS Surface Water Scenarios.

Before the TOXSWA model can be run TOXSWA needs project information defined in SWASH and a *.m2t or *.p2t output file from MACRO or PRZM, respectively. Guidance is given in the SWASH User's

guide (Fait *et al.*, 2013) and in the MACRO and PRZM manuals (Appendices J and K of FOCUS, 2001). Therefore, before being able to run TOXSWA for FOCUS scenarios, SWASH, MACRO and PRZM need to be installed and run. Below an overview is given of all steps in SWASH, MACRO and PRZM that are necessary to create, open and run a FOCUS Step 3 project in TOXSWA:

1. Start SWASH.
2. Define the substance or select an already defined substance from the SPIN database (connection automatically from SWASH).
3. Use the FOCUS wizard to define a project for the specified substance and crops you wish to consider.
4. Press 'View Projects and Define Applications' and fill in the relevant application pattern (by editing the given default application pattern if necessary) and check all other run specifications.
5. Press the button 'Export FOCUS input to MACRO, PRZM and TOXSWA' with all options selected.
6. Print the project report.
7. Click on the MACRO button on the upper bar of the SWASH main window to start the MACRO shell, SWASH remains in the task bar.
8. Run MACRO for all D scenarios listed in the project report. Do not forget to create the *.m2t output files after having finished the MACRO runs; they are automatically stored in the correct directories.
9. Exit the MACRO shell and enter SWASH again.
10. Click on the PRZM button on the upper bar of the SWASH main window to start the PRZM shell and SWASH closes.
11. Run PRZM for all R scenarios listed in the project report. The *.p2t files are automatically prepared during the PRZM runs and placed in the correct directories.
12. Exit the PRZM shell and enter SWASH again.
13. No action is needed to calculate the spray drift deposition onto the water body: SWASH prepares this value automatically, when you click the button 'Export FOCUS input to MACRO, PRZM and TOXSWA'.
14. Click on the TOXSWA button on the upper bar of the SWASH window to start the TOXSWA shell, and the SWASH shell closes.
15. You will now enter the 'TOXSWA – Projects' window from where you can proceed.

4.4.1 Running TOXSWA

In the TOXSWA GUI the project can be opened by selecting the project and pressing the OK button, or by double-clicking on the project. A new window with all the runs in the project appears. By default, all runs in the project have been selected for execution.

1. You can switch runs on and off by double-clicking in the column 'Selected'.

You may want to check that the *.m2t or *.p2t files are already in the correct directories: to do so, select a run and press the button 'View input file' on the status bar. In Section 7 Management section, in table *Soil substance files* the path and name of the *.m2t or *.p2t input file is given. Check with the aid of the Windows explorer if the correct *.m2t or *.p2t input file is available at the specified location.

Now, press the calculate button to run the model. A form pops up where you can select the run options. See section 4.4.11 for the explanation of the different options. Then:

1. All selected runs will be carried out
2. The TOXSWA GUI will write the input files and if selected call the simulation kernel.
3. You can follow the progress of the simulation in the DOS-box on your screen or run it in the background without screen output.

After completion of a run, at the TOXSWA project window, in the 'Browse Runs' table under the header 'Results', you will see the message 'Not available' change to 'Available' or to 'Error' in case errors have been encountered during the run.

1. If errors are encountered, you will see that the Report and Graphs buttons have been disabled.
2. The nature of the error can be learned from the error file. Press 'View' and then 'Error file' in the status bar to display the error file on the screen.
3. Errors can also be viewed in the Run Status tab of the main form.

Note that the time steps and segment lengths are defined in such a way that a convergent and stable solution is expected. However, the responsibility for convergence of the numerical solution is to the user. Furthermore, the numerical solution can become unstable for (combinations of) extreme parameterisations. It is known that for low (0.7) and high values (1.2) used for the Freundlich exponent combined with high sorption coefficients the solutions might become unstable. This is shown by errors indicating errors in the mass balance or indicating that positivity conditions are not fulfilled. In those cases it is advised to the numerical discretization (i.e. shorten the segment lengths) and/or shorten time steps (see also Section 4.4.3).

4.4.2 Viewing the results

Press the Report button to view the FOCUS report. This report contains, amongst others:

1. An overview of the applications and pesticide entries of the two entry routes: spray drift and drainage or runoff/erosion.
2. The Global Maximum Concentration in water and in sediment.
3. TWAECs, Time-Weighted Average Exposure Concentrations in water and in sediment over pre-defined periods.

Press the Graph predefined button to view graphs of

1. Concentration of pesticide in water as a function of time
2. Concentration of pesticide in sediment as a function of time
3. Mass balance of pesticide in water layer
4. Mass balance of pesticide in sediment
5. Distribution of pesticide between the various compartments

Note that output of relevant data must be selected before calculation.

Press the Graph user defined button to view the predefined graphs (see above) and graphs of

6. Hydrology: discharge from upstream, between segments and downstream
7. Hydrology: water depth
8. Hydrology: drainage flux, runoff flux
9. Mass fluxes: drainage, runoff and erosion'
10. Sediment concentrations as a function of depth and of time

Note that output of relevant data must be selected before calculation (doornummeren??).

4.4.3 Special cases: substances with K_{oc} higher than 30000 L/kg

The TOXSWA GUI selects the standard FOCUS segmentation with 14 segments in the sediment for FOCUS locations (Section 4 of the *.txw input file of Annex 2). For substances with a K_{oc} of less than 30000 L/kg this results in a stable and converging numerical solution of the mass conservation equations, and consequently to correct exposure concentrations in water and sediment. For substances with a K_{oc} higher than 30000 L/kg, e.g. pyrethroids, the numerical solution does not converge for the sediment nor for the water layer, i.e. the calculated concentrations in the sediment and in the water layer depend on the size of the segments in the sediment. Therefore, the GUI selects the FOCUS_highKoc sediment segmentation with 23 segments for FOCUS Step 3 runs with substances with K_{oc} values above 30000 L/kg (see Annex 4 for the Sediment section of the TOXSWA input file with segmentation and sediment properties for this case). This is indicated by a pop-up message that appears when the calculate button is pressed for a project that contains this type of runs. The message has to be clicked away by the user to continue. For non-FOCUS Step 3 projects, the message is also given, but the FOCUS-highKoc sediment segmentation is not selected automatically. The user can change the sediment segmentation. To do so, copy the relevant location at the Locations form. In this copied location, exchange the FOCUS sediment for the FOCUS-highKoc sediment. Go back to the Main form, select the run and replace the location by the location with FOCUS-highKoc sediment. Then the run can be executed. However, it remains the responsibility of the user to check that he/she has indeed obtained a converging solution with this proposed segmentation.

4.4.4 Special cases: metabolite formation in water of upstream catchment of FOCUS streams

FOCUS_TOXSWA 4.4.2 simulates the formation of metabolites in water and in sediment. A consequence of this new functionality of TOXSWA for the FOCUS scenarios is to account for metabolites formed in the upstream catchment that enter the downstream water body. This is not needed for FOCUS ditches and ponds as these scenarios do not have upstream fields treated with pesticides. For FOCUS streams 20 ha of the 100-ha upstream catchment are treated with pesticides. Therefore, the FOCUS stream scenarios are the only FOCUS scenarios needing input of metabolite mass across the upstream boundary of the stream.

Adriaanse *et al.* (2014) describe how to calculate the correction factor that accounts for metabolite formation in the upstream catchment of FOCUS streams. Only metabolites formed in the water layer of the upstream catchment are considered. The same correction factor, $CF_{m,up}$, accounts for:

1. Metabolite formation in the upstream catchment from parent mass entered by spray drift deposition from the 20 ha treated fields and
2. Metabolite formation in the upstream catchment from parent mass originating from runoff or drainage from the 20 ha treated fields.

In the GUI the correction factor $CF_{m,up}$ needs to be entered as "Fraction primary metabolites formed in water in upstream catchment", which can be found at the Edit runs form at the Entries tab in the section upstream catchment entries (see Fig. 4.3).

The screenshot shows the 'Edit Run' window with the 'Entries' tab selected. The 'Drainage or Runoff' section includes a dropdown for 'Type' set to 'Runoff', a 'File name' field with a file path, a 'Model' dropdown set to 'PRZM', a 'Loading fluxes' dropdown set to 'Hourly', and a 'Thickness sediment layer' field set to '0.01'. The 'Runoff' section has a 'Fraction infiltrating, draining to waterbody (0-1):' field set to '0.1'. The 'All entries' section has 'Start position (m):' set to '0' and 'End position (m):' set to '100'. The 'Upstream catchment entries' section has 'Ratio of upstream catchment treated (0 - 1):' set to '0.2' and 'Fraction primary metabolites formed in water in upstream catchment (0 - 1):' set to '1'.

Figure 4.3 Entries tab of the Edit runs form. The section Upstream catchment entries contains the correction factor $CF_{m,up}$, that accounts for metabolite formation in the water layer of the upstream catchment.

The correction factor needs to be calculated by the user according to the description given in Appendix 2 of Adriaanse *et al.* (2014). Note that:

- a. The factor is only valid for primary metabolites, i.e. metabolites formed directly from the parent,
- b. The correction factor is metabolite-specific. As TOXSWA can handle one correction factor only, this means that, if more than one (primary) metabolite is formed, more TOXSWA simulations are needed, one for each metabolite,
- c. The correction factor is scenario-specific, because its value is a function of the water temperature and of the residence time in the upstream catchment of the scenario.

The entry of this factor for FOCUS Step 3 runs will be automated by SWASH in its next release. As long as this is not yet done a default value of 1 is set by the GUI, i.e. a conservative estimate.

4.5 General properties of the TOXSWA GUI

All windows of the TOXSWA GUI have a similar set-up, which will be explained in this section. The Runs form is taken as an example. The form consists of two parts: (i) a browse box, shown in Figure 4.4, and (ii) an edit section with option fields, shown in Figure 4.5.

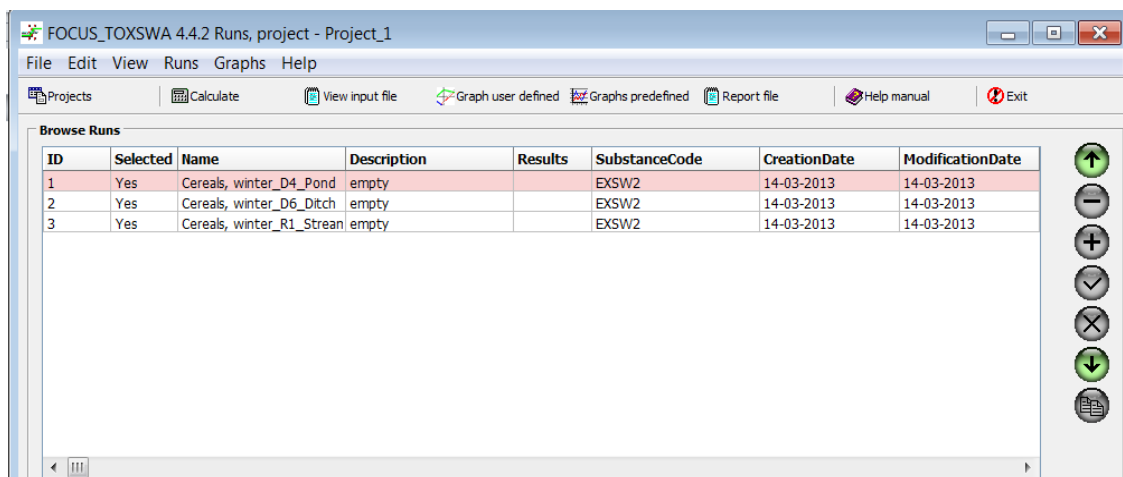









Figure 4.4 The browse box of the Runs form.

The browse box allows the user to scroll through the records of a table (in this example, runs). The information in the edit box in the lower half of the screen (Figure 4.5) changes when scrolling. All browse boxes are complemented with a navigator, consisting of:

-  go to the first item/run in the browse runs table
-  delete the run selected
-  create a new run
-  save the changes made by the user
-  cancel the changes made by the user
-  go to the last item/run in the table
-  copy the selected run

Buttons are displayed in green when active (their function is allowed) or in grey when inactive (the function is presently not allowed and unavailable). For instance when a record has not yet been edited, then the buttons 'Save changes' and 'Cancel changes' are grey instead of green.

Edit Run

Run Components | Entries | Simulation Control | Output Control | Run Status | Comment

Name: Cereals, winter_D4_Pond

Description: empty

Scenario

Location: D4_Pond

Crop: Cereals, winter

Pesticide and Scenario

Substance: EXSW2

Application scheme: AppScheme_1

Initial conditions for pesticides

Initial concentration water layer (mg/L): 0

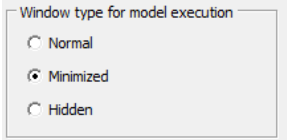
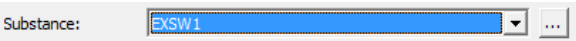
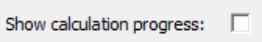
Initial content sediment...

Figure 4.5 The edit box of the Runs form.

In the edit box of a form the user can edit the record selected in the browse box.

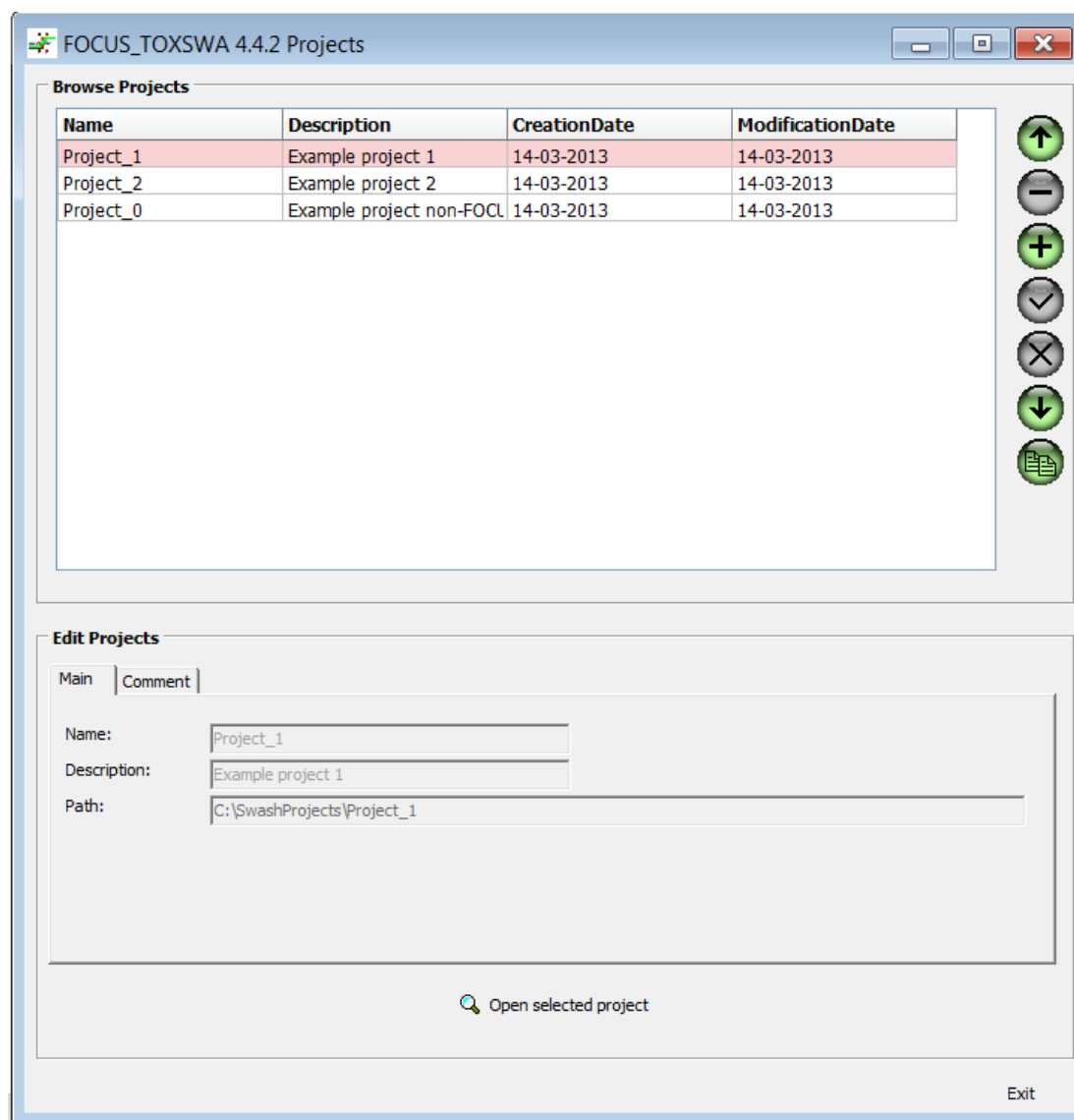
The TOXSWA GUI employs four categories of data fields:

- ordinary data fields (e.g.), where the user can enter a text string, a data string, or numerical data. The TOXSWA GUI will perform range checking after entry of the data.

- radio buttons (e.g. ), where the user can select only one of the shown options.
- pick lists (e.g., ) where the user can make a choice between a number of options. The button to the right of a pick list (a square with three dots) allows the user to edit the underlying tables (i.e. go to a lower hierarchical level).
- check boxes (e.g. ) where the user can switch options on or off.

4.6 Projects form

The 'Projects' form appears after starting the TOXSWA GUI. The Projects form allows you to organize your runs into projects (Figure 4.6). A project is a set of runs, usually for one substance (and its metabolites when present) with one or several crops. Each run is characterised by a location, substance and application scheme.



Name	Description	CreationDate	ModificationDate
Project_1	Example project 1	14-03-2013	14-03-2013
Project_2	Example project 2	14-03-2013	14-03-2013
Project_0	Example project non-FOCL	14-03-2013	14-03-2013


Edit Projects

Main | Comment

Name:

Description:

Path:

 Open selected project

Exit

Figure 4.6 The Projects form of the TOXSWA GUI.

Entirely new projects can be created with the aid of the FOCUS wizard in SWASH or the user-defined wizard in SWASH. In the TOXSWA GUI existing projects can be copied and altered or a new project can be created with the + navigator button. The first column 'Name' gives the name of the project, the second column 'Description' allows for a short description of the project. The last two column 'CreationDate' and 'ModificationDate' specify the date the project was created and modified for the last time, resp.

In this upper part of the window, a browse box, the user can select a project with the aid of the navigator. The navigator allows the user to jump to the first project, to jump to the last project, to create a project or delete a project, respectively. The copy button allows the user also to make a copy of the selected project. By pressing the 'Open selected project' button at the bottom of the window the selected project is opened. This can also be achieved by double clicking on a project. When a project is opened, the Runs form is entered, and the name of the selected project is shown in the title bar of the Runs form.

Via the Comment tab comments to the project can be written in the white box. This option is available only for projects that are created or copied in the TOXSWA GUI.

On the right hand bottom end of the window the user is offered the option to leave the TOXSWA GUI by pressing the 'Exit' button.

4.7 Runs form – TOXSWA project: project_name

The Runs form appears after selecting a project and pressing the 'Open selected project' button (or double clicking on the project) in the Projects form. The title bar of the Runs form displays the name of the selected TOXSWA project (Figure 4.7).

ID	Selected	Name	Description	Results	SubstanceCode	CreationDate	ModificationDate
1	Yes	Cereals, winter_D4_Pond	empty		EXSW2	14-03-2013	14-03-2013
2	Yes	Cereals, winter_D6_Ditch	empty		EXSW2	14-03-2013	14-03-2013
3	Yes	Cereals, winter_R1_Stream	empty		EXSW2	14-03-2013	14-03-2013

Edit Run

Run Components | Entries | Simulation Control | Output Control | Run Status | Comment

Name: Cereals, winter_D4_Pond

Description: empty

Scenario

Location: D4_Pond

Crop: Cereals, winter

Pesticide and Scenario

Substance: EXSW2

Application scheme: AppScheme_1

Initial conditions for pesticides

Initial concentration water layer (mg/L): 0

Initial content sediment...

Figure 4.7 The Runs form of the TOXSWA GUI.

This form is the central point from where the different tables of the database can be accessed, the model runs can be started and graphs from the TOXSWA output can be viewed. The status bar (bar at the top of the form) or the buttons at the form can be used to navigate through the GUI.

The lower half of the main form consists of six tabs, i.e. a Run Components tab, an Entries tab, a Simulation Control tab, an Output Control tab, a Run Status tab, and a Comment tab. These tabs are described in more detail in Sections 4.7.4 to 4.7.9.

4.7.1 Status bar of the Runs form

The status bar contains six menus (File, Edit, View, Runs, Graphs, and Help) which will guide the user to different processes. Clicking each of these menus will show a grey box with options for different processes. Table 4.1 explains all options.

Table 4.1

Options on the Status Bar on the Runs form of the TOXSWA GUI

Option	Sub option	Action
File:	Close	Closes the GUI
Edit:	Projects	Return to the Projects form
	Locations	Opens the Locations form
	Substance	Opens the Substances form (in SPIN)
	Application Schemes	Opens the Application Schemes form
	Initial conditions for pesticides	Opens the Initial conditions for pesticide
View:	View input File	Opens the input file (*.txw)
	Report File	Makes and opens the report file: excerpt of summary output file (*.sum)
	Summary file	Opens the summary output file (*.sum)
	Log file	Opens the echo file (*.ech)
	Error file	Opens the error file (*.err)
Runs:	Select all runs	All runs will be selected ('Yes' in browse runs boxes)
	Deselect all runs	All runs will be deselected (browse runs boxes are blanked)
	Delete output of selected run	Removes the output of a selected run in the browse box
Graphs	Graphs user defined	Opens the 'Detailed output options' form
	Graphs predefined	Opens the 'Choice of predefined graphs' form
Help	Help manual	Opens the TOXSWA user manual document
	TOXSWA website	Opens TOXSWA's homepage on http://www.PesticideModels.eu
	Whats new	Opens a document describing the new added features
	About	Shows details on development

4.7.2 Main buttons of the Runs form

The functions of the main buttons below the status bar of the Runs form are described in Table 4.2.

Table 4.2

Main buttons of the Runs form of the TOXSWA GUI

Button	Action
Projects:	Return to the Projects form
Calculate:	Starts the calculations of all the runs selected in the browse box
View input file:	Opens the TOXSWA input file (*.txw)
Graphs user defined:	Opens the Detailed output options form
Graphs predefined:	Opens the Choice of predefined graphs form
Report file:	Makes and opens the report file of the runs
Help manual	Opens the TOXSWA user manual document
Exit	Allows the user to leave the TOXSWA GUI

By clicking on the Report file button the GUI makes and displays a report of the selected run. This report is an excerpt of the summary output file. This report is not saved automatically. The user can select and copy the content of the report to a file (e.g. in Notepad) whilst the report is on display.

4.7.3 Browse box of the Runs form

The column 'ID' in the Browse runs section shows the runID of the run, which consist of numbers.

For a run prepared in SWASH that includes drainage entries, and which has e.g. a TOXSWA runID of 4, the matching runID's of MACRO output files are:

Parent: macro00004_p.m2t

if there is one soil metabolite:

Metabolite 1: macro00004_m.m2t

or if there are two soil metabolites:

Metabolite 1: macro00004_m_1.m2t

Metabolite 2: macro00004_m_2.m2t

For a run prepared in SWASH that includes runoff entries, and which has e.g. a TOXSWA runID of 5, the matching runID's of PRZM output files are:

Parent: 00005_C1.p2t

if there is one soil metabolite:

Metabolite 1: 00005_C2.p2t

and if there is also a second soil metabolite:

Metabolite 2: 00005_C3.p2t

The difference is the result of differences in naming the output file between MACRO and PRZM. MACRO can handle only one metabolite in one simulation resulting in the _m.m2t file. For two metabolites MACRO needs two simulation runs, and after in the conversion of MACRO output to m2t files, ID's are assigned in such a way that the IDnrs correspond to the runID of TOXSWA (managed by SWASH). PRZM can handle two metabolites in one simulation run, and does not need additional procedures.

In the Browse runs section, the user can select a run by clicking on the run. If a run is selected the column 'Selected' shows the word 'Yes', otherwise this column entry is blank. The navigator allows the user to jump to the first run, delete a run, create a run, accept changes, discard changes or to jump to the last run, resp. Moreover, the 'Copy' button allows the user to make a copy of the selected run.

The column 'Name' shows the name of the run and the column 'Results' shows whether output is available. When a simulation has not yet been done the column 'Results' is blank. If a run has been performed successfully the column 'Results' will show the message 'Available'. If a run did stop during the simulation because of an error, the column 'Results' shows the message 'Error'. The nature of the error can be learned from the message on the Run Status tab.

The column 'Locked' shows whether a record is locked, i.e. whether it can be edited or not. All records in the Browse runs section that have been prepared by SWASH i.e. FOCUS Step 3 runs, are locked in the TOXSWA GUI. The whole project is locked. To change the properties, the project needs to be copied. FOCUS Step 4 runs can be set up by combining items that were made by SWASH, e.g. combining a substance with another application scheme. Another possibility is to set up runs from items that have been made by the user in the separate forms.

4.7.4 Run Components tab

The 'Run components' tab of the Runs form contains the sections *Scenario*, *Pesticide and Scenario* and *Initial conditions for pesticides* (Figure 4.8).

The 'Name' field shows the name of the run. When the run has been prepared by SWASH (FOCUS Step 3), the name is a combination of the crop, scenario and water body names.

The user has to select the major run components of a run, i.e. Scenario Location, the Pesticide and Scenario dependent characteristics Substance and Application scheme, and Initial conditions for the pesticide. For projects containing FOCUS Step 3 runs, all run components are automatically selected and filled with the correct input data.


Notice that you can only select existing components in this form. It may be necessary to add or create entirely new locations composed of entirely new components. In this case you can use the button on the right of the pick list () to go to a lower hierarchical level, where you can e.g. compose new locations or new substances.

Figure 4.8 Run Components tab of the Runs form.

Scenario

The 'Location' field gives access to the water layer (including hydrology), sediment layer, and meteo station components of the run. For projects prepared with SWASH the 'Crop' field shows a crop name because the FOCUS runs have been set up for a specific crop. When these projects are copied in the TOXSWA GUI the crop name is also copied and shown. For projects created in the TOXSWA GUI this field is empty, because TOXSWA inputs are not crop dependent. The box 'Crop' is grey, so a crop cannot be entered or changed. This field has been added in the TOXSWA GUI to inform the user for which crop the pesticide entries via spray drift deposition and drainage or runoff/erosion have been generated with SWASH (FOCUS Step 3 run).

Pesticide and Scenario

The 'Substance' field gives access to the SPIN tool, where the physico-chemical properties of the substance, i.e. general properties and sorption and transformation parameters can be entered, edited and managed. The 'Application scheme' field gives access to data on the applications and the spray drift entries.

Initial conditions for pesticides

In the 'Initial conditions for pesticide...' box the initial concentrations in the water layer and in the sediment are specified.

4.7.5 Entries tab

The Entries tab contains the sections Drainage or Runoff, Runoff, All entries and Upstream catchment entries.

Drainage or Runoff

The user can indicate whether drainage or runoff entries have to be simulated via the Pick box 'Type'. The file name, including its path (table Soil substance files²), of the file containing the drainage or runoff fluxes needs to be specified (Figure 4.9). The small button at the end of this line allows to user to browse through his folders in order to locate the correct lateral entry route file. The Loading fluxes item (OptInp) gives the choice between either hourly or daily fluxes. The latter option is not operational in FOCUS_TOXSWA_4.4.2. Therefore these options are greyed out. The thickness of the sediment layer to which pesticide mass sorbed to eroded soil is added (ThiLayErs) needs to be entered for runoff runs, where erosion is simulated as well.

Either drainage or runoff, or neither, is simulated. When lateral entries are simulated the file with lateral fluxes needs to be selected. For FOCUS Step 3 scenarios the MACRO model provides the entries via drainpipes and the PRZM model the entries via runoff and erosion. The MACRO *.m2t output files lists water and pesticide fluxes leaving drainpipes on an hourly basis. The PRZM *.p2t output files lists water and pesticide runoff fluxes plus additional columns with eroded soil, pesticide mass adsorbed to eroded soil and water fluxes infiltrating, all at an hourly basis. Not simulating lateral entries means that there are no lateral water (and associated pesticide) fluxes entering the water body. The file name option field shows 'empty' in this case.

When lateral entries have to be simulated, a variable hydrology in the water body is assumed. The appropriate hydrology needs to be selected at the Water body page.

Runoff

The fraction of infiltrating water draining into the water body (RatInfDir) can be given. This for the ratio of pesticide-free infiltrated water at 1 depth that drains directly into the water body.

All entries

The start (Start of stretch of watercourse loaded by all loading types) and end positions (End of stretch of watercourse loaded by all loading types) in the water body, in between which drift deposition and drainage or runoff take place need to be specified.

Upstream catchment entries

The ratio of the upstream catchment that is treated with the pesticide (RatAreaUpsApp) has to be entered. This is relevant for waterbodies with upstream catchments, i.e. watercourses, not for ponds. Furthermore the fraction primary metabolites formed in water in the upstream catchment (FraMetForUps) can be entered. This is only relevant if primary metabolites formed in water are simulated, and the ratio of upstream catchment treated is not zero.

The screenshot shows the 'Edit Run' dialog box with the 'Entries' tab selected. The 'Drainage or Runoff' section contains the following fields: 'Type' (Runoff), 'File name' (D:\SwashProjects\CProject_2\PRZM\cereals_winter\00092-C1.p2), 'Model' (PRZM), 'Loading fluxes' (Hourly), and 'Thickness sediment layer, to which mass sorbed to eroded soil is added (m)' (0.01). The 'Runoff' section contains the field 'Fraction infiltrating, draining to waterbody (0-1)' (0.1). The 'All entries' section contains the fields 'Start position (m)' (0), 'End position (m)' (100), 'Ratio of upstream catchment treated (0 - 1)' (0.2), and 'Fraction primary metabolites formed in water in upstream catchment (0 - 1)' (1).

Figure 4.9 Entries tab of the Runs form; drainage calculated with the MACRO model.

² Names in courier letter type refer to the name of the variable in the TOXSWA input file

4.7.6 Simulation Control tab

This tab page contains general options for controlling the simulation run in the sections *Simulation period* and *Calculation time steps* (Figure 4.10).

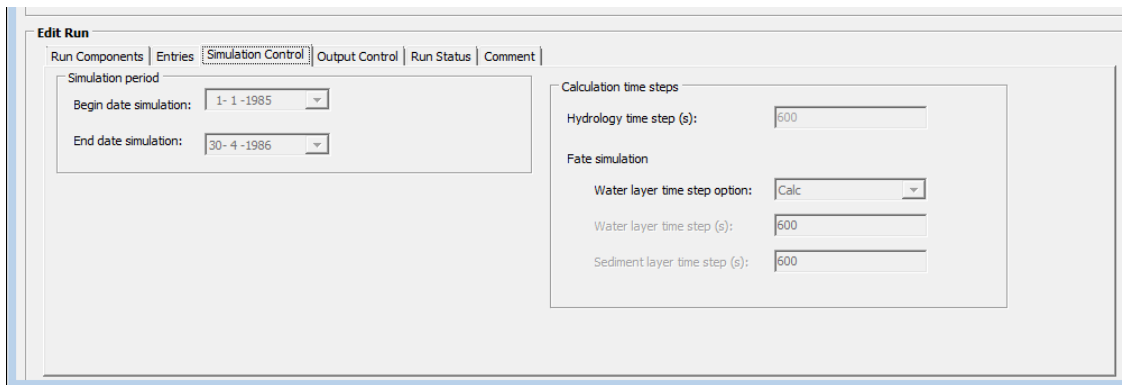
The screenshot shows the 'Edit Run' window with the 'Simulation Control' tab selected. The 'Simulation period' section contains two date pickers: 'Begin date simulation' set to '1-1-1985' and 'End date simulation' set to '30-4-1986'. The 'Calculation time steps' section includes a text input for 'Hydrology time step (s)' with the value '600'. Below it, the 'Fate simulation' section has a dropdown for 'Water layer time step option' set to 'Calc', and two text inputs for 'Water layer time step (s)' and 'Sediment layer time step (s)', both with the value '600'.

Figure 4.10 Simulation Control tab of the Runs form.

Simulation period

The time-domain for the simulation is specified by the user entering a start date ($TimStart$) and an end date of the simulation ($TimEnd$). Dates are input in the format dd-mm-yyyy (e.g. 30-01-2002).

Calculation time steps

The calculation time steps for the hydrology can be entered ($TimStpHyd$). The default value is 600 s. For the fate simulation (solve the mass balance) two time step options ($OptTimStp$) are available: fixed time steps set by the user ('Input'), and calculation of the time steps ('Calc'). For the option 'Input' the calculation time steps for water layer ($TimStpWat$) and for the sediment layer ($TimStpSed$) can be entered. The default value is 600 s for both time steps. For the option 'Calc' the calculation time step to solve the mass balance for the water layer and the sediment are selected by TOXSWA itself. They vary between 1 and 3600 s, depending on the flow dynamics. Using this option, the maximal values of both time steps need to be assigned ($MaxTimStpWat$ and $MaxTimStpSed$). This is not possible in this version of the GUI.

4.7.7 Output Control tab

The 'Output Control' tab of the Main TOXSWA form (Figure 4.11) contains the section *General*, and a button to access the 'Detailed output options' of the run. The detailed output options are described in 4.11.

Furthermore, the 'Depth of target layer' can be entered ($ThiLayTgt$), indicating the thickness of the top layer of the sediment for which the exposure concentrations in sediment are calculated.

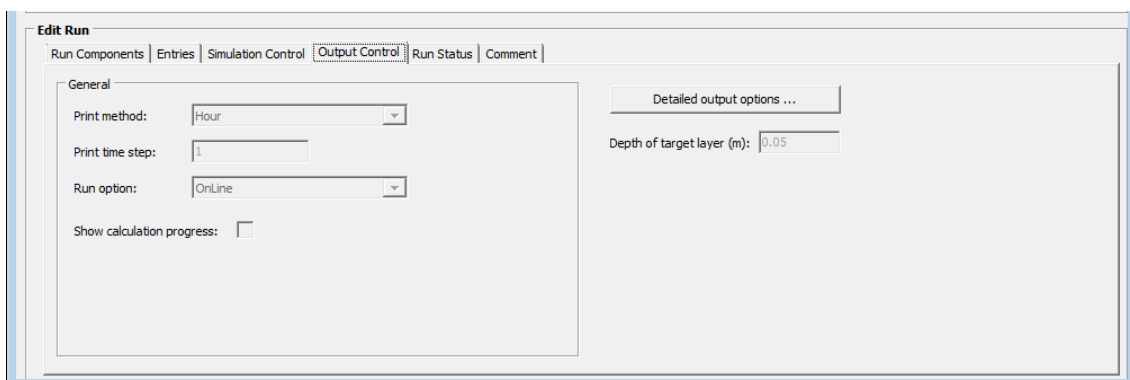
The screenshot shows the 'Edit Run' window with the 'Output Control' tab selected. The 'General' section contains four controls: 'Print method' (dropdown set to 'Hour'), 'Print time step' (text input with '1'), 'Run option' (dropdown set to 'OnLine'), and 'Show calculation progress' (checkbox). To the right of these controls is a button labeled 'Detailed output options ...'. Below the button is a text input for 'Depth of target layer (m):' with the value '0.05'.

Figure 4.11 Output Control tab of the Runs form.

General

The 'Print method' (`OptDelTimPrn`) in combination with the 'Print time step' (`DelTimPrn`) specifies the Output time interval. The default value for the time interval is 1 hour, which is also the minimum output time interval. *Notice that the output of TOXSWA is averaged over the print interval and that the time printed is in the middle of the print interval.* The size of the output file can be reduced by setting the output interval to higher values. Note that, when the output time interval is set to values larger than 1 hour, the graphs will show results for this larger time interval. So, e.g. a global maximum concentration that occurs between the start and end time of the interval is not shown in the graph. Nevertheless, the summary report file reports the actual global maximum and its time of occurrence.

In the 'Run option' field (`OptHyd`) the user can indicate if hydrology as well as mass balance need to be calculated, or only the hydrology, or only the mass balance. The default option is: Run hydrology and then substance. For more details about the run option see Section 3.3.4 of this report.

The option 'Show calculation progress' (`OptScreen`) is not operational in FOCUS_TOXSWA 4.4.2.

The 'Depth of target layer' (`ThiLayTgt`) indicates over which depth the concentrations in sediment are averaged in the output of TOXSWA.

4.7.8 Run Status tab

The Run Status tab page presents the date the run was created as well as the date that it was modified for the last time. The error file (*.err) is created during the run. If no error occurs during the run, the file is removed at the end of the run. If the run stops due to an error, the content of the error file is displayed in the right hand side of the Run Status tab (Figure 4.12).

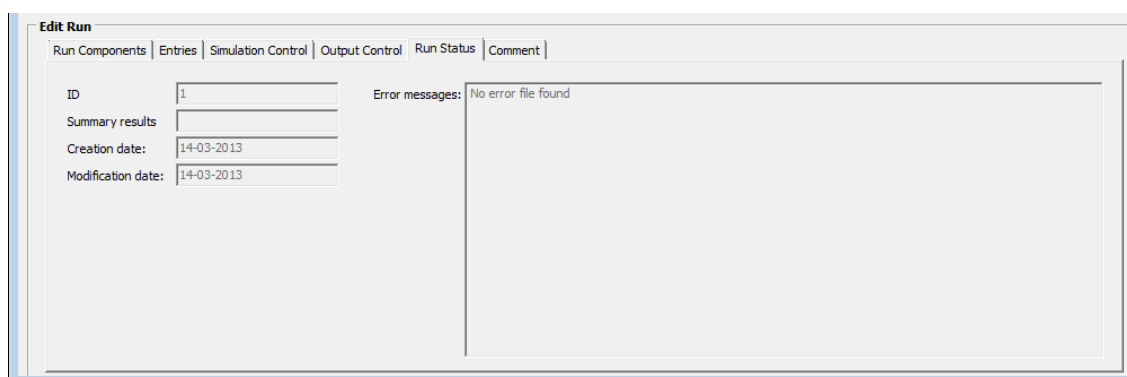


Figure 4.12 Run Status tab of the Runs form.

4.7.9 Comments tab

This tab allows the user to add comments or meta-data concerning the selected run in a text box.

4.8 Editing Locations

From the Locations form (Figure 4.13) the user can view and select the components of the location, and access some general data of the locations.

A new location can be added with the + button of the navigator or an existing location can be copied. The FOCUS locations cannot be changed. After pressing the + button, in the appearing insert box, the user must specify a unique code for the location (`Location`). The country name (not required) can be specified.

Furthermore the user has to select a water layer, a sediment layer and a meteo station. Please note that it may be necessary to create e.g. a new water layer and/or e.g. new sediment before you can select one. Then, you have to add these items at the Water layer, Sediment and Meteo station forms before proceeding.

The longitude, latitude and altitude of the scenario location may be specified (not required); note that the meteo station may be located elsewhere; this can be specified at the Meteo stations form (Section 4.8.3).


The seepage rate ($FlwWatSpg$), expressed in mm/d of the contributing neighboring plot, and the concentration in the incoming upward seepage water ($ConWatSpg$) may be specified. In FOCUS_TOXSWA 4.4.2, the seepage options are not used.

Name	Description	Country	Water Layer	Sediment	Meteostation
D1_Ditch	D1 Ditch (meteostation Lanna)		D1_DITCH	FOCUS	Lanna
D1_Stream	D1 Stream (meteostation Lanna)		D1_STREAM	FOCUS	Lanna
D2_Ditch	D2 Ditch (meteostation Brimstone)		D2_DITCH	FOCUS	Brimstone
D2_Stream	D2 Stream (meteostation Brimstone)		D2_STREAM	FOCUS	Brimstone
D3_Ditch	D3 Ditch (meteo station: Vredepeel)		D3_DITCH	FOCUS	Vredepeel
D4_Pond	D4 Pond (meteo station: Skousbo)		D4_POND	FOCUS	Skousbo
D4_Stream	D4 Stream (meteo station: Skousbo)		D4_STREAM	FOCUS	Skousbo
D5_Pond	D5 Pond (meteo station: La Jailliere)		D5_POND	FOCUS	La_Jailliere
D5_Stream	D5 Stream (meteo station: La Jailliere)		D5_STREAM	FOCUS	La_Jailliere
D6_Ditch	D6 Ditch (meteo station: Thiva)		D6_DITCH	FOCUS	Thiva
R1_Pond	R1 Pond (meteo station: Weiherbach)		R1_POND	FOCUS	Weiherbach
R1_Stream	R1 Stream (meteo station: Weiherbach)		R1_STREAM	FOCUS	Weiherbach
R2_Stream	R2 Stream (meteo station: Porto)		R2_STREAM	FOCUS	Porto
R3_Stream	R3 Stream (meteo station: Bologna)		R3_STREAM	FOCUS	Bologna
R4_Stream	R4 Stream (meteo station: Roujan)		R4_STREAM	FOCUS	Roujan

Name:	<input type="text" value="D4_Pond"/>	Longitude (dec. degrees, East positive):	<input type="text" value="0"/>
Description:	<input type="text" value="D4 Pond (meteo station: Skousbo)"/>	Latitude (dec. degrees):	<input type="text" value="0"/>
Country:	<input type="text"/>	Altitude (m):	<input type="text" value="0"/>
Water Layer:	<input type="text" value="D4_POND"/> ...	Seepage flux (mm/d):	<input type="text" value="0"/>
Sediment Layer:	<input type="text" value="FOCUS"/> ...	Concentration in seepage (mg/L):	<input type="text" value="0"/>
Meteo Station:	<input type="text" value="Skousbo"/> ...		

Figure 4.13 The Locations form.

4.8.1 The Water layers form

The Water layers form can be accessed by pressing the  button behind the pick list of the option field 'Water layer' in the Locations form.

In the Water layers form (Figure 4.14) a water layer has to be defined, by specifying a name ($WaterbodyID$) and choosing a Hydrology Type (combination of $OptWaterSystemType$ and $OptFloWat$). The possible hydrology types are WaterCourse, Pond and Constant. Values can be attributed to the different parameters defining the water layer.

A new water layer can be added with the + button of the navigator or an existing water layer can be copied. The water layers form presents 4 tabs (General, Watercourse, Pond, Constant). The General tab is accessible independent of the type of Hydrology Type. Of the other 3 tabs, the user can only enter data on the tab corresponding to the Hydrology Type chosen.

General tab

At the General tab of the Water layers form the user can:

- Change the dimensions i.e. 'Length of water layer' (Len), bottom width (WidWatSys) and side slope (SloSidWatSys) of the water body, and edit the number of segments within the water layer (NumSeg).
- Change the depth-defining perimeter (DepWatDefPer) indicates the water depth that defines the length on the sidewalls across which the substance in the water interacts with the sediment. Above this water depth there is no exchange of substance between water and sediment.
- Change some water layer characteristics: concentration suspended solids (ConSus) and the mass ratio of organic matter of the suspended solids (CntOmSusSol) and dry weight of the macrophytes per m² bottom area (AmaMphWatLay).

Browse WaterLayer

Name	Hydrology type	BottomWidth	NumberOfSegments	TotalLength
R1_POND	Pond	30	1	30
D1_DITCH	WaterCourse	1	10	100
D1_STREAM	WaterCourse	1	20	100
D2_DITCH	WaterCourse	1	10	100
D2_STREAM	WaterCourse	1	20	100
D3_DITCH	WaterCourse	1	10	100
D4_STREAM	WaterCourse	1	20	100
D5_STREAM	WaterCourse	1	20	100
D6_DITCH	WaterCourse	1	10	100
R1_STREAM	WaterCourse	1	20	100
R2_STREAM	WaterCourse	1	20	100
R3_STREAM	WaterCourse	1	20	100
R4_STREAM	WaterCourse	1	20	100
Vredepeel_ditch	WaterCourse	0.5	10	100

Edit WaterLayer

Name: Hydrology Type:

General | Watercourse | Pond | Constant

Length water layer (m)::	<input type="text" value="100"/>	Depth defining perimeter (m):	<input type="text" value="0.1"/>
Bottom Width (m):	<input type="text" value="0.5"/>	Concentration suspended solids (mg/L):	<input type="text" value="15"/>
Number of segments:	<input type="text" value="10"/>	Mass ratio organic matter:	<input type="text" value="0.5"/>
Side slope (hor/ver):	<input type="text" value="1"/>	Macrophytes dry weight (g/m2):	<input type="text" value="0"/>

Close

Figure 4.14 The Water layers form, with the General tab opened on the bottom half.

Note that TOXSWA simulates a trapezium-shaped sediment system (see Adriaanse, 1996). However, if both the side slope of the water body is zero and the water depth defining perimeter is zero, TOXSWA simulates only the vertical column of sediment below the water layer. Such a vertical column equals the situation in artificial systems as e.g. mesocoms and water-sediment test systems (see the example in Section 5.1).

Watercourse tab

Figure 4.15 shows the Watercourse tab in the lower part of the Water layers form. On the left side of the tab parameters for the watercourse are given. On the right side of the tab the section *Representative channel* with parameters for the representative channel are given. The form for a

watercourse type hydrology shows option fields in which you can enter the constant 'Base flow' ($Q_{BasWatCrsInp}$), the 'Upstream area' ($Area_{UpsWatCrsInp}$) delivering its water (and sometimes pesticide fluxes) into the watercourse, the 'Width plot along watercourse' (Wid_{FldDra} for drainage, Wid_{FldRnf} for runoff) contributing drainage or runoff fluxes (water and pesticide) and 'Margin erosion' (Wid_{FldErs}) contributing pesticide sorbed onto eroded soil fluxes to the watercourse.

The dispersion coefficient option (Opt_{Dis}) can be set. If the option is 'Input', the dispersion coefficient, constant during the simulation, must be entered as well. If the option is 'Fischer', the dispersion coefficient is calculated from the flow velocity and dimensions of the watercourse. If the option is constant, the value of the 'Dispersion coefficient' ($Cof_{DisPhsInp}$) must be entered. When the flow is variable, use of Fischer is recommended.

Figure 4.15 The Watercourse tab of the Water layers form.

Representative channel

The characteristics of the representative channel (Figure 4.15) represent the average conditions for a watercourse in the catchment considered: channel 'Length' (Len_{RepCha}), 'Bottom slope' ($Slo_{BotRepCha}$), 'Bottom width' of the channel ($Wid_{BotRepCha}$), 'Side slope' ($Slo_{SidRepCha}$), constant 'Base flow' ($Q_{BasRepCha}$), the 'Upstream area' of the catchment ($Area_{UpStrRepCha}$), 'Weir height' of the weir crest above the channel bottom of the channel ($Hgt_{CreRepCha}$), 'Weir width' i.e. crest width of the weir located at the outflow of the channel ($Wid_{CreRepCha}$), 'K-Manning'; bottom roughness at 1 m water depth (Cof_{RghRef}) and 'Alpha', the energy coefficient, resulting from the non-uniform distribution of flow velocities over a channel cross section (Cof_{VelHea}).

The representative channel is used to calculate the variation of the water level as a function of time in TOXSWA's watercourse for the discharge coming out of the upstream catchment basin. More information about the representative channel can be found in Section 2.1 of this report or in Adriaanse and Beltman (2009).

Pond tab

Figure 4.16 shows the Pond Tab in the lower part of the Water layers form.

In this form values can be entered for the 'Contributing area' of the pond ($Aera_{SurPndInp}$), the 'Base flow' into the pond ($Q_{BasePndInp}$), the 'Height' and 'Width' of the weir (Hgt_{CrePnd} , Wid_{CrePnd}) controlling the outflow of the pond and the area from which erosion, 'Area erosion', may enter the pond ($Area_{ErsSurPndInp}$). The contributing area of the pond corresponds to the area surrounding the pond that delivers its water and pesticide fluxes into the pond. The pond hydrology does not need a representative channel, whilst watercourses do.

Edit WaterLayer

Name: Hydrology Type:

General | Watercourse | **Pond** | Constant

Contributing area (ha):

Base flow (m3/d):

Height weir (m):

Width weir:

Area erosion (ha):

Close

Figure 4.16 The Ponds tab of the Water layers form.

Constant tab

Figure 4.17 shows the Constant Tab in the lower part of the Water layers form.

The hydrology type 'Constant' offers the user the possibility to enter 'Flow velocity' ($Vel_{WatFlwBas}$), 'Water depth' (Dep_{Wat}) and the type of 'Dispersion' (see explanation given for Watercourse tab) for systems with a constant waterflow. Selecting this type of hydrology type is useful when e.g. simulating results for a water-sediment system. For the hydrology type constant, the definition of an upstream catchment is not necessary.

Edit WaterLayer

Name: Hydrology Type:

General | Watercourse | Pond | **Constant**

Flow velocity (m/s):

Water depth (m):

Dispersion:

Dispersion coefficient (m2/d):

Figure 4.17 The Constant tab of the Water layers form.

4.8.2 The Sediment form

The Sediment form can be accessed by pressing the  button behind the pick list of the option field 'Sediment layer' in the Locations form.

The Sediment form consists of two parts. The left half of the form (Browse Sediment) contains entire sediments. A sediment consists of several sediment layers. In the right half (Browse sediment layer) properties of individual sediment layers can be edited.

In the Edit Sediment section on the left side of the Sediment form (Figure 4.18) a sediment has to be defined, by specifying a 'Name' (*SedimentTypeID*). A description can be added. Furthermore, it should be indicated whether the 'Sediment properties' (*OptSedProperties*) are all given as input, or the porosity is to be calculated from the other properties (see explanation in section 3.3.7). For more details about the estimation of sediment properties see also Annex 6.

In the Browse sediment section a new sediment can be added with the + button of the navigator or an existing sediment can be copied.

In the Browse sediment layers section on the right side of the Sediment form the layers of the sediment are defined. The sediment consists of a number of layers (named horizons in txw file and in Section 3.3.7), which on their turn are composed of segments. The properties of each layer are defined by the selected Building Block. In the Edit sediment layers section the user can modify the different layers by specifying the 'Sub layer no.' (*Nr*), the 'Sediment Building block code', the 'Thickness' (*ThiHor*) of the layer and the 'Number of segments' (*NumLay*) in the layer. A new sediment layer can be added with the + button of the navigator or an existing sediment layer can be copied.

Figure 4.18 The Sediment layers form.

Building blocks form

It may be necessary to create new sediment building blocks or to edit an existing building block. To achieve this, the user has to enter the Building Blocks form via the pick list behind the 'Sediment Building Block code' option field³.

The 'Building blocks' form (Figure 4.19) contains the 'Browse buildingblocks' table showing all building blocks in the database and the 'Edit buildingblocks' section where the data of the building block can be entered or edited.

A new building block can be added with the + button of the navigator or an existing building block can be copied and edited.

³ Note that after a new sediment has been added, and the user wants to define new building blocks for this sediment, the GUI gives an error (List index out of bounds (-1)). Click OK, and then first add a sediment layer in the right part of the form, to which temporarily an existing building block must be attributed. Alternatively, the user can first define new building blocks, and thereafter add the sediment with its sediment layers.

For each building block values need to be entered for the 'Dry bulk density' ρ_b (Rho), 'Porosity' ε (ThetaSat), 'Tortuosity' λ (CofDifRel), 'Mass ratio organic matter' $m_{om,wb}$ (CntOm), and 'Dispersion length' (LenDisSedLiq).

Browse buildingblocks

Name	BulkDensity	Porosity	Tortuosity
FOCUS-SB1	800	0.6	0.6
Vredepeel-SB1	80	0.82	0.82
Vredepeel-SB2	220	0.77	0.77
Vredepeel-SB3	670	0.77	0.77
Vredepeel-SB4	1500	0.36	0.28

Edit buildingblocks

Name:

Dry bulk density (kg/m3):

Porosity:

Tortuosity:


Mass ratio of organic matter (kg/kg):

Dispersion length (m):

Close

Figure 4.19 The Building blocks form.

4.8.3 The Meteo stations form

The Meteo Stations form (Figure 4.20) can be accessed by pressing the  button behind the pick list of the option field 'Meteo Station' in the Locations form.

The Browse Meteo Stations section at the upper half of the window gives an overview of all available locations with meteorological data. At present TOXSWA only needs data concerning the water body temperature. For the FOCUS scenarios monthly values of the air temperature are used in the TOXSWA simulations.

The lower half of the window presents details of the selected meteorological station. The only obligatory field is the Caption field (note that Caption is used here, while in the Browse table Name is used) (MeteoStation), all other fields are optional. The longitude, latitude and altitude of the location of the meteo station may be specified; note that the scenario to be simulated may be located elsewhere; this can be specified at the Locations form (Section 4.7.1).

The three buttons at the right hand of the form offer various possibilities with respect to the meteorological data file. The View Data button allows the user to inspect the used data on his screen.

The Create Datafile button creates from the selected meteo data the meteo file (*.met) in the TOXSWA directory of the project that the user is working in. Note that creating the meteo file is not needed to perform a run. When in the Main form the Calculate button is pressed, the *.met file is created automatically.

Browse Meteostations

Name	Description	StartDate	EndDate
Bologna	Bologna	01-01-1975	31-12-1994
Brimstone	Brimstone	01-01-1975	31-12-1994
La_Jailliere	La Jailliere	01-01-1975	31-12-1994
Lanna	Lanna	01-01-1980	31-12-1993
Porto	Porto	01-01-1975	31-12-1994
Roujan	Roujan	01-01-1975	31-12-1994
Skousbo	Skousbo	01-01-1975	31-12-1994
Thiva	Thiva	01-01-1977	31-12-1994
Vredepeel	Vredepeel	01-01-1975	31-12-1994
Weiherbach	Weiherbach	01-01-1975	31-12-1994

Edit Meteostations

Caption:

Description:

Country:

Longitude (dec. degrees, East positive):

Latitude (dec degrees):

Altitude (m):

View data ...

Create Datafile

Import Datafile ...

Close

Figure 4.20 The Meteo Stations form.

The Import Datafile button allows the user to import new meteorological data into the SWASH/TOXSWA database under the selected Meteo Station Name. The new Meteo Station Name must have been created first with the aid of the Copy or + button at the Browse Meteo Stations section. It is possible to import a new set of meteo data into the TOXSWA/SWASH database by creating a data file of identical layout as the TOXSWA *.met files in the SWASH projects directory. The name of the file and the name in the header of the meteo file (behind 'Weather station') have to correspond with the caption entered for the new meteo station in the GUI (see Figure 4.21). Press the Import Datafile button, confirm by pressing Yes to the question that pops up (see Figure 4.22). Next, locate the file with defined meteo data with the Windows Explorer, open it, and the TOXSWA GUI reads its content and puts it into the SWASH/TOXSWA database.

FOCUS_TOXSWA 4.4.2 MeteoStations

Browse Meteostations

Name	Description	StartDate	EndDate
Bologna	Bologna	01-01-1975	31-12-1994
Brimstone	Brimstone	01-01-1975	31-12-1994
La_Jailliere	La Jailliere	01-01-1975	31-12-1994
Lanna	Lanna	01-01-1980	31-12-1993
Porto	Porto	01-01-1975	31-12-1994
Roujan	Roujan	01-01-1975	31-12-1994
Skousbo	Skousbo	01-01-1975	31-12-1994
Thiva	Thiva	01-01-1977	31-12-1994
Vredepeel	Vredepeel	01-01-1975	31-12-1994
Weiherbach	Weiherbach	01-01-1975	31-12-1994
Test		01-01-1970	01-01-1970

Caption/name should be the same as the name of the weather station specified in the meteorology file behind '* Weather station:'

Edit Meteostations

Caption:
 Description:
 Country:
 Longitude (dec. degrees, East positive):
 Latitude (dec degrees):
 Altitude (m):

Close

Figure 4.21 The meteo stations form for the example water-sediment study.

Confirm

Important:
Importing meteo data will erase any existing data for the selected meteo station

Make sure the name behind the "Weather station:" in the header of the meteo data file you are importing, has already been defined in the GUI on the TOXSWA Meteo stations form

Also make sure the format of the file that will be imported equals the format of the TOXSWA *.met file


Don't use tabs or commas, and remove all empty lines from the file.

Do you want to proceed importing data ?

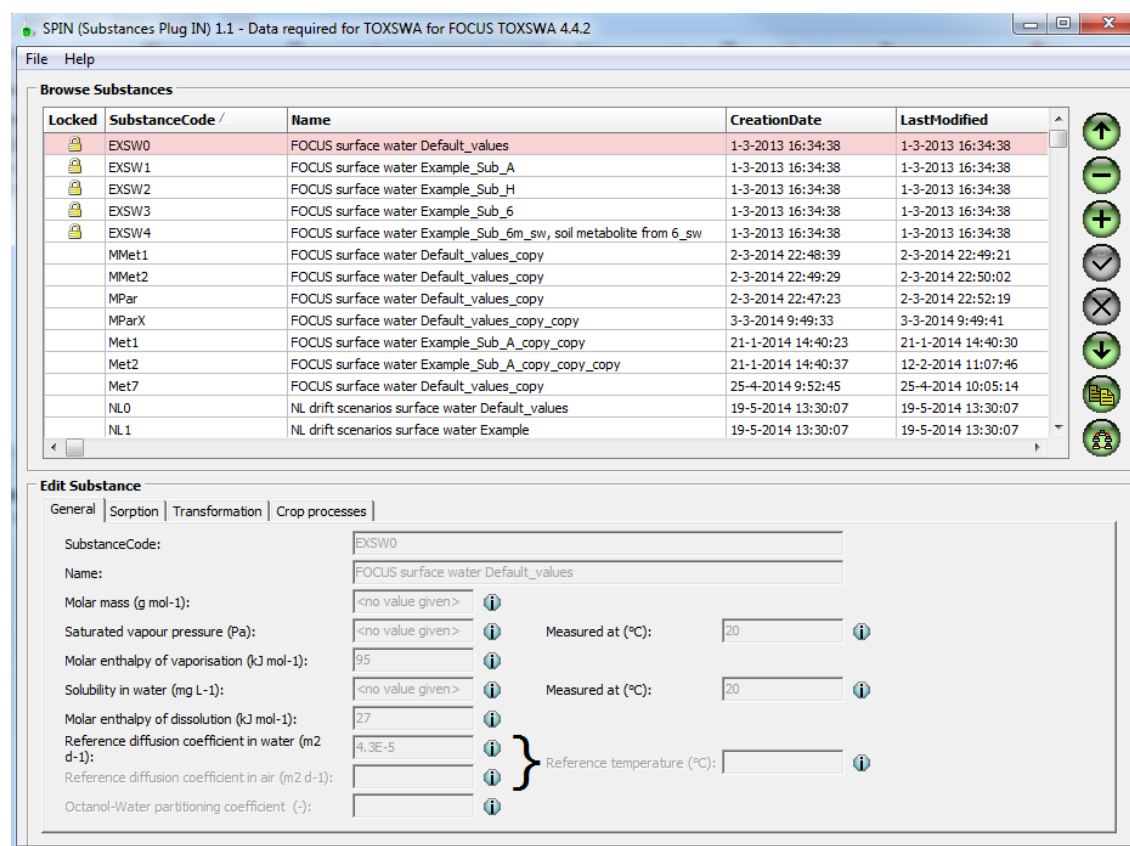
Figure 4.22 Window with instructions shown after pressing the button 'Import Datafile ...' in the Meteo Stations form.

4.9 Editing substances

The Substances form is accessible from the Run Components tab of the Runs form.

Press the  button behind the pick list of the option field 'Substance' in the Runs form. Alternatively, the user may choose the 'Edit Substance' from the menu bar in the Projects form.

This opens the SPIN (Substances Plug IN) program, enabling the user to add and/or edit substances (Figure 4.23). For details about defining and editing substances from within SPIN the user is referred to the SPIN manual (van Kraalingen *et al.*, 2013), which can also be accessed via the SPIN GUI.



Browse Substances

Locked	SubstanceCode /	Name	CreationDate	LastModified
	EXSW0	FOCUS surface water Default_values	1-3-2013 16:34:38	1-3-2013 16:34:38
	EXSW1	FOCUS surface water Example_Sub_A	1-3-2013 16:34:38	1-3-2013 16:34:38
	EXSW2	FOCUS surface water Example_Sub_H	1-3-2013 16:34:38	1-3-2013 16:34:38
	EXSW3	FOCUS surface water Example_Sub_6	1-3-2013 16:34:38	1-3-2013 16:34:38
	EXSW4	FOCUS surface water Example_Sub_6m_sw, soil metabolite from 6_sw	1-3-2013 16:34:38	1-3-2013 16:34:38
	MMet1	FOCUS surface water Default_values_copy	2-3-2014 22:48:39	2-3-2014 22:49:21
	MMet2	FOCUS surface water Default_values_copy	2-3-2014 22:49:29	2-3-2014 22:50:02
	MPar	FOCUS surface water Default_values_copy	2-3-2014 22:47:23	2-3-2014 22:52:19
	MParX	FOCUS surface water Default_values_copy	3-3-2014 9:49:33	3-3-2014 9:49:41
	Met1	FOCUS surface water Example_Sub_A_copy_copy	21-1-2014 14:40:23	21-1-2014 14:40:30
	Met2	FOCUS surface water Example_Sub_A_copy_copy_copy	21-1-2014 14:40:37	12-2-2014 11:07:46
	Met7	FOCUS surface water Default_values_copy	25-4-2014 9:52:45	25-4-2014 10:05:14
	NL0	NL drift scenarios surface water Default_values	19-5-2014 13:30:07	19-5-2014 13:30:07
	NL1	NL drift scenarios surface water Example	19-5-2014 13:30:07	19-5-2014 13:30:07

Edit Substance

General | Sorption | Transformation | Crop processes

SubstanceCode:

Name:

Molar mass (g mol⁻¹):

Saturated vapour pressure (Pa): Measured at (°C):

Molar enthalpy of vaporisation (kJ mol⁻¹):

Solubility in water (mg L⁻¹): Measured at (°C):

Molar enthalpy of dissolution (kJ mol⁻¹):

Reference diffusion coefficient in water (m² d⁻¹):

Reference diffusion coefficient in air (m² d⁻¹):


Octanol-Water partitioning coefficient (-):

Reference temperature (°C):

Figure 4.23 View of substances in SPIN database.

4.10 Editing Application schemes

The Application schemes and applications form is accessible from the Run Components tab of the Runs form.

The Application scheme and applications form can be accessed by pressing the  button behind the pick list of the option field 'Application scheme' on the Run Components tab. In the Application Scheme form information about the applications and spray drift can be entered.

The left hand part of the form concerns the applications schemes, and the right hand part concerns the individual applications in the selected applications scheme (Figure 4.24).

In the left hand upper part of the form, the Browse application scheme section, with various applications schemes is shown. Application schemes can be added with the + button of the navigator or an existing application scheme can be copied. An unique name (ApplicationScheme) has to be entered in Edit application schemes section.

The right hand upper part of the form shows the Browse applications section with the one or more individual applications that are joined together into the selected application scheme. In application schemes that are not defined in SWASH, individual applications can be edited, or applications can be added to the application scheme using the + button or the copy button of the navigator.

When adding an application to an application scheme, the user has to enter an 'Application number', the 'Dosage' used, the 'Drift percentage' appropriate for the application, and the 'Date of application'.

Three entry routes to the water body are considered in TOXSWA; spray drift, drainage and runoff/erosion. The spray drift is entered here in the Application schemes form. The relevant data for drainage and runoff/erosion are entered at the 'Entries' tab of the Runs form.

Browse application schemes

Name
Default_Scheme
AppScheme_1
AppScheme_3
AppScheme_5
AppScheme_6
Vredepeel
AppScheme_4
AppScheme_2

Browse applications

Appl. nr	Dosage	Drift perc.	Appl. date
1	1	0.154	30-12-1899
2	0.75	0.154	30-12-1899
3	0.5	0.154	30-12-1899

Edit application schemes

Name: AppScheme_1

Edit applications

Application number: 1

Dosage (kg/ha): 1

Drift percentage (%): 0.154

Date of application: 30-12-1899

Close

Figure 4.24 The Application scheme form.

The drift percentage may be defined by the user or calculated with the FOCUS drift calculator (Appendix H; FOCUS, 2001). The user has to enter the value for the drift percentage manually in the option field, except for FOCUS Step 3 scenarios, where the complete Application scheme form and applications are automatically filled in, because they are defined in SWASH.

Note that TOXSWA uses the water depth to convert the mass deposited per m² water surface to mass entering per running meter water body, by multiplying the mass deposited per m² with the cross section of the water layer ($b + 2 \cdot h \cdot s_1$). Due to the rectangular shape of the FOCUS water bodies ($s_1 = 0$), this multiplication does not affect the FOCUS runs.

If the application scheme is defined by SWASH (FOCUS Step 3 run), the date fields are dummy values. TOXSWA receives the application dates from the header of the MACRO *.m2t file or from the PRZM *.p2t file. The MACRO or PRZM model has determined the exact application date with the aid of the Pesticide Application Timer (PAT) and within the application window specified in SWASH (see Section 4.2.6 of FOCUS, 2001). The TOXSWA model checks that the input specified in the TOXSWA GUI with respect to number of applications and dosage corresponds to those mentioned in the header of the *.m2t or *.p2t file. If no drainage or runoff input is used (de facto; constant flow simulations), the dates of application cannot be read from the MACRO or PRZM output files because they are not part of the simulation, so dates of application have to be entered in the TOXSWA GUI.

4.11 Running the model

The model simulations have to be done from the Runs form, which shows all the runs in the selected project in its Browse box. By default, all runs in the project are selected for execution. By double-clicking a run in the Browse box, the run is deselected for execution, and vice versa. When deselecting a run, the 'Selected' indicator will no longer contain 'Yes', but will turn blank. If you want to select (or deselect) all runs in the project, select (or deselect) all runs by clicking 'Runs' in the status bar in the Runs form and then click 'select all runs' (or 'deselect all runs'). The 'Runs' entry in the Runs status bar also enables the user to delete output previously generated for the selected run (select 'Delete output of selected run').

After having checked that all input is correct, the run can be started. A powerful feature of the TOXSWA GUI is that it is possible to execute multiple runs in series, and therefore it is not necessary to wait until the first run has finished before starting the second run. When all desired runs are selected, the 'Calculate' button can be pressed to run the model.

Every time the 'Calculate' button is pressed, the TOXSWA GUI will generate the TOXSWA input files and meteo data files of the files selected for execution. This can take some time. Be aware that this also means that when the input files were changed outside the GUI, those changes are lost because the GUI recomposes the input files and the edited input files are overwritten!

Prior to the start of calculations, the user is offered a number of options with regard to the output generated, as well as some options with respect to the calculations themselves on the Multiple run options form shown in Figure 4.25.

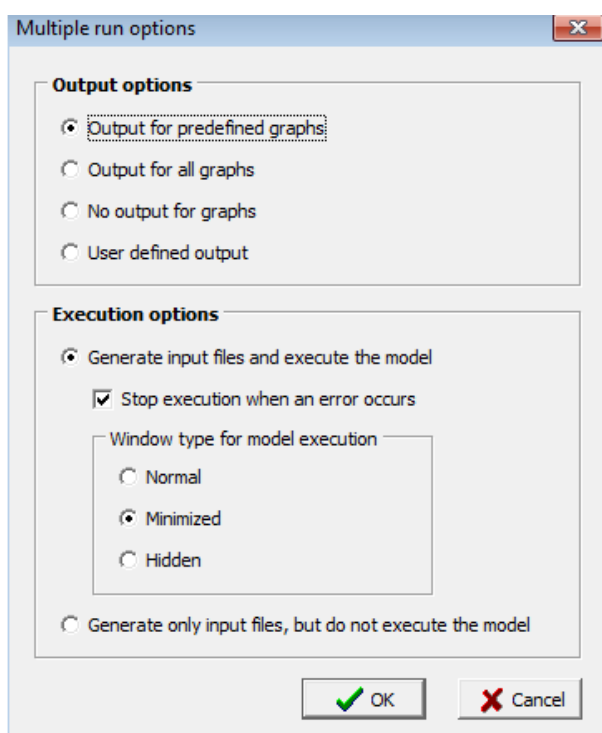


Figure 4.25 Output and execution options offered by TOXSWA when starting a run.

The user may define which output will be created by TOXSWA. The summary file is always generated. The additional data generated (in the *.out file) for each choice are:

- Output for predefined graphs: for main graphs as described in section 4.12.2.
- Output for all graphs: to be able use all graphs possible in GUI.
- No output for graphs
- User defined output: see options described in section 4.11.2.

If the option 'User defined output' is used, the options have to be set before the button Calculate is pressed, for each run.

The user may define whether the runs are executed (option 'Generate input files and execute the model'), or only input files are written (option 'Generated only input files, but do not execute the model'). This second option is available for expert users that do large series of runs without using the GUI for execution of the model.

If the runs are to be executed the calculations can be stopped when an error occurs by ticking the box 'Stop execution when an error occurs'. When this box is not ticked and an error occurs during a run, the model will continue the calculations with the next run.

Three Window types are available for visualisation during the execution of the runs. If the 'Window type' is set to Normal, a console window will be shown. The user can monitor the progress of the simulation in this window. If Minimized is selected, the console window is available on the task bar and the window can be set to normal. If Hidden is selected, the window accompanying the calculations will not be shown at all. Use the CTRL-C option of the keyboard of the pc to interrupt the model execution. The actual computation time depends mainly upon the number of numerical segments in the water layer and the length of the period simulated. To give an indication: execution of the FOCUS stream scenario for winter cereals in Skousbo took about 2.5 minutes on an Intel i5-2520M CPU, 2.50 GHz computer with memory size 4 GB. Computation time can be reduced by reducing the number of output files to be written or reducing the number of output segments. FOCUS ditch and pond scenarios require considerably less computation time.

When a model run is completed, the value in the 'Results' column in the Browse runs box in the Run form will change from blank into 'Available' or into 'Error' if errors were encountered during the run. The nature of the error can be retrieved from the error file. View the Run Status tab of the Main form, or press 'View' and then 'error file' in the status bar to display the error file on the screen. When errors were encountered, the Reports and Graphs buttons will be disabled.

Before running the model, you have to define the output that you want to create with TOXSWA. However, the default settings of the TOXSWA user interface have been set so that you usually don't need to bother about output control. Output is controlled via the output tab of the runs form, and is explained in section 4.7.7. When at the Multiple run options form the option 'user defined output' is used, options selected on the Detailed output options forms are used for the simulations (see section 4.12).

4.12 Editing detailed output options

The detailed output options form is accessible from the output control tab of the Runs form (Figure 4.26).

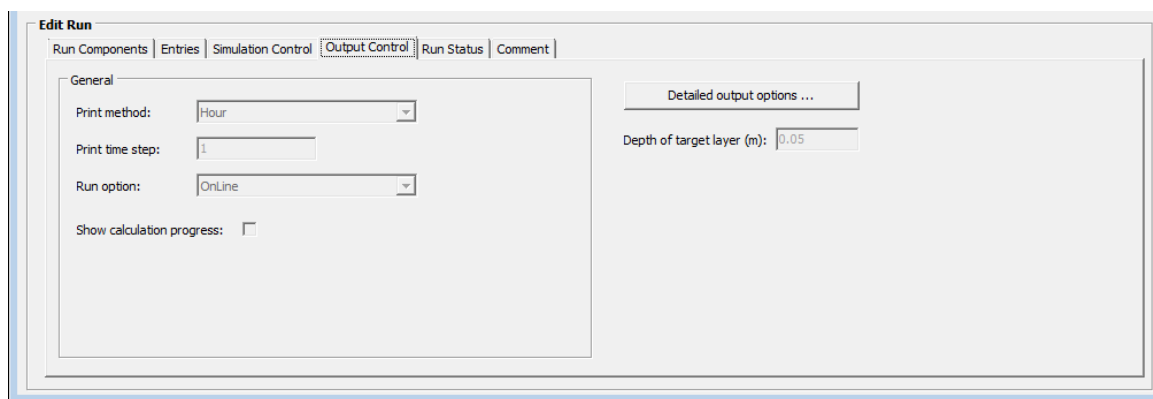


Figure 4.26 The output control tab of the Runs form, with the 'Detailed output options' button on the right side of the tab.

The Detailed output options form (Figure 4.27) consists of three parts:

- In the upper part the categories of available variables can be browsed.
- In the lower part the individual variables within a category can be browsed (and selected by double clicking on the 'Selected' column of a variable). For each variable is shown whether output can be generated as a function of distance (indicated in column 'HasDistance') and/or as a function of depth in sediment (indicated in column 'HasDepth').
- In the upper right part of the form the user can select and browse, if applicable, the distances for output of water and sediment variables (i.e. position along the length of the water body) and for sediment, the depths of output for sediment variables (i.e. depth in sediment). The selection made here is applied to all variables in all categories that have been selected for output.

Figure 4.27 The detailed output options form.

The categories of variables available for output are:

- Hydrology: discharge in water body⁴, drainage and runoff fluxes, and the depth of the water layer.
- Mass balance water layer: balance including e.g. mass in water layer, mass entered by spray drift, and mass transformed in water layer.
- Mass balance sediment layer: balance including e.g. mass in sediment layer, mass entered from water layer, and mass transformed in sediment layer.
- Mass fluxes: drainage, runoff, and erosion substance fluxes entering the water body.
- Concentrations: concentrations as a function of time in water and in sediment (averaged in depth).
- Sediment concentrations: concentrations in sediment as a function of time, of distance and of depth.
- Distribution: distribution of mass between liquid and sorbed phases in water and in sediment.
- <no graphs available for this variable>: variables that can be set as output, but are not used for graphs that can be made by the GUI.

⁴ Note that in the graphs the distance is given in reference to the middle of the segment. However, the discharge concerns the discharge at the lower boundary of the segment, i.e. for the pond (defined as 1 segment of 30 m long), the distance indicated in the graph is 15 m, whereas the discharge in the output file of TOXSWA concerns the discharge at 30 m.

At the bottom of the form three buttons are available that manage all output of TOXSWA. Pressing 'Clear all variables' disables the output for all variables, pressing 'Set all variables' sets the output for all variables, and pressing 'Set predefined' sets TOXSWA to generate the output for the predefined graphs (see section 4.13.2).

For the distances and depths boxes in the upper right part, using the + button of the navigator will allow the user to add additional output distances and/or depths. The selection should be saved, by using the 'Ok' button prior to leaving the distances or depths box.

4.13 Creating graphs

4.13.1 Predefined graphs

After a model run has been completed, the output can be analysed via the graphical function of the FOCUS_TOXSWA GUI. FOCUS_TOXSWA can prepare a number of pre-defined graphs (see Figure 4.28). They represent the most important model outputs, such as the concentration of pesticides in the water body, content in sediment, the mass balance of the substance in the water layer etc. The right hand box enables the selection of compounds for which the graphs are prepared, allowing the user e.g. to choose between a parent compound and one or more of its metabolites. The predefined graphs are accessed through the 'Graphs predefined' button in the Runs form.

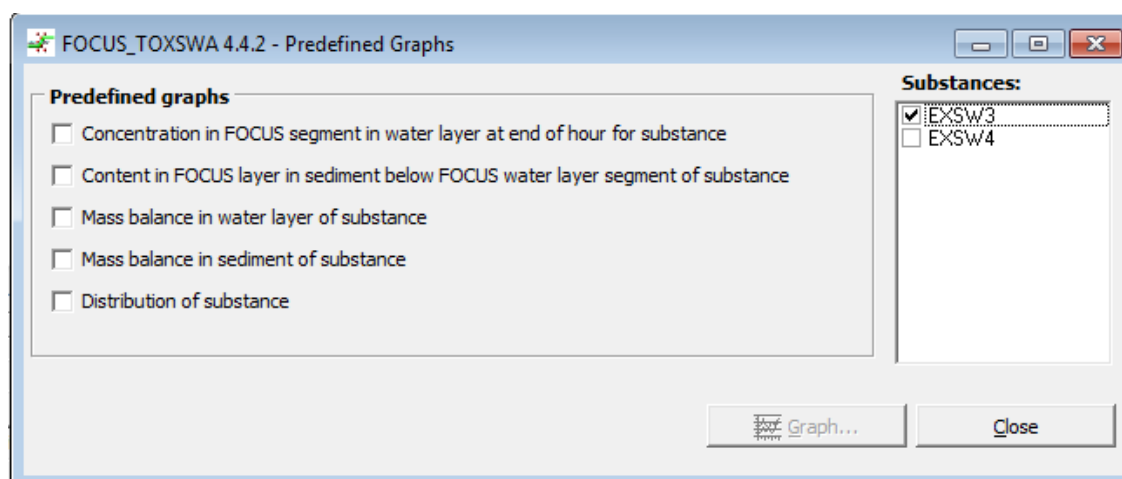


Figure 4.28 Choosing from predefined graphs.

4.13.2 User defined graphs

The user is also allowed to create his own graphs, enabling him to view the data in additional ways. Graphs can be prepared for any of the variables selected in the Detailed output options (see section 4.12). The user defined graphs can be accessed with the 'Graph user defined' button in the Runs form, allowing the user to choose from the variables selected in the Detailed output options.

TOXSWA can create graphs of all selected model outputs (section 4.12). The custom graphs form is accessed from the Runs form. To create a graph, perform the following actions:

- Select one of the categories in the upper box.
- Select one or more variables by double clicking the variable name in the lower box.
- If the selected variable is distance or depth dependent, select one or more distances or depths by clicking in the appropriate boxes on the right hand side.
- If the selected variables are substance properties, the user can select one or more substances in the substances box.

FOCUS_TOXSWA 4.2.2 uses an embedded graphical program (TeeChart) to display graphs. After the graph is displayed (see e.g. Figure 4.29) the user can zoom in by selecting part of the graph while keeping the left mouse button pressed, moving down and to the right, and releasing it after the

desired section of the graph has been selected. To zoom out to the original size of the graph, do the same, but move up and left. The 'Print' and 'Save' options in the menu bar of the graph enable printing and saving of the graph. The 'Edit' menu buttons offer options to customize the graph. On the 'Edit' form help to change the graph can be accessed via clicking the 'Help' button.

4.13.3 Demonstration of some graphs

To demonstrate the graphical features of FOCUS_TOXSWA 4.4.2, three graphs are shown, presenting simulation results of the example substance EXSW3.

The concentration in the FOCUS segment in the water layer is shown in figure 4.29. The pesticide concentration in the FOCUS segment of the water layer in the last segment of the watercourse at the end of the hour is shown. The concentration at the end of the hour is shown, which we mention explicitly, because all other output is shown as the average of the time step of output (mostly 1 hour). However in hourly averaged values of concentrations the peak concentrations due to spray drift events would not be visible in the graphs, because spray drift is a instantaneous event.

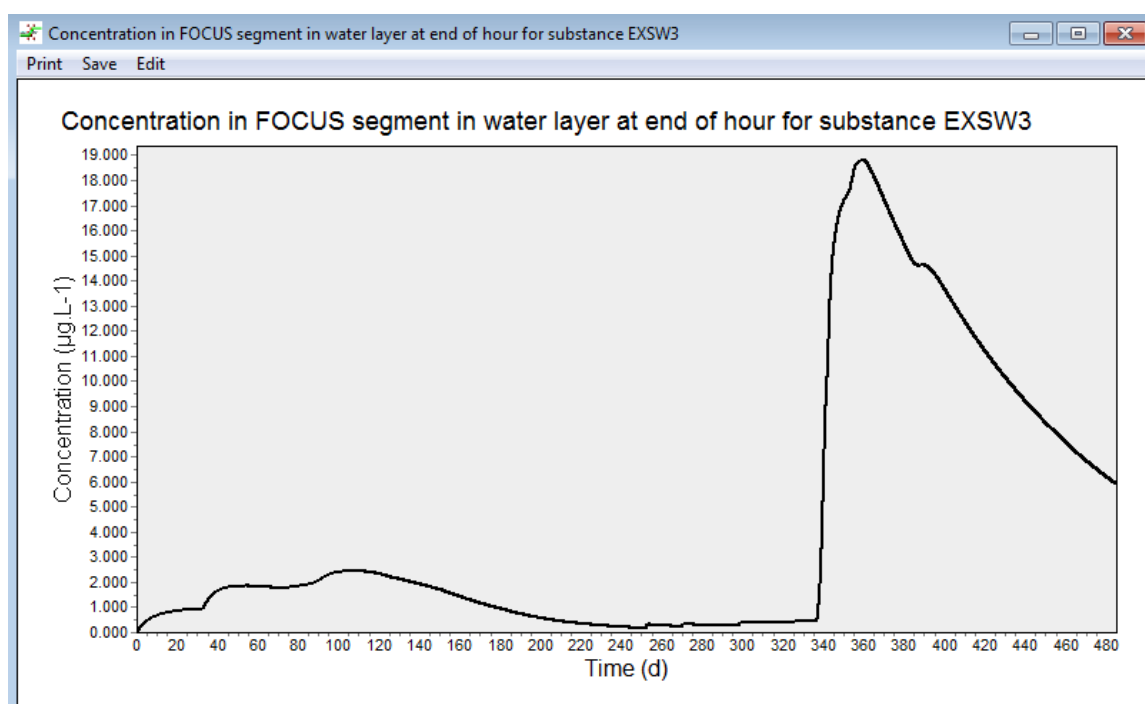


Figure 4.29 TOXSWA graph: Concentration of pesticide in the FOCUS segment of the water layer as a function of time.

The mass balance of the water layer is shown in figure 4.30. The red curve ('Remaining') shows the mass of the substance that is present in the system as a function of time. All other curves give the cumulative of change as a function of time. Variables marked with '+' indicate how much mass has come into the water layer, e.g. the top purple line indicates the cumulative mass that has entered the water layer via drainage. Variables marked with '--' indicate the cumulative mass that has gone out of the water layer, e.g. the green line indicates the cumulative mass that has left to the sediment layer.

All mass balance terms of substance EXSW3 for the entire water layer are shown in the figure. By selecting and deselecting the appropriate terms in the check boxes in the legends on the right hand side of the graph, the user may select which mass balance terms are shown.

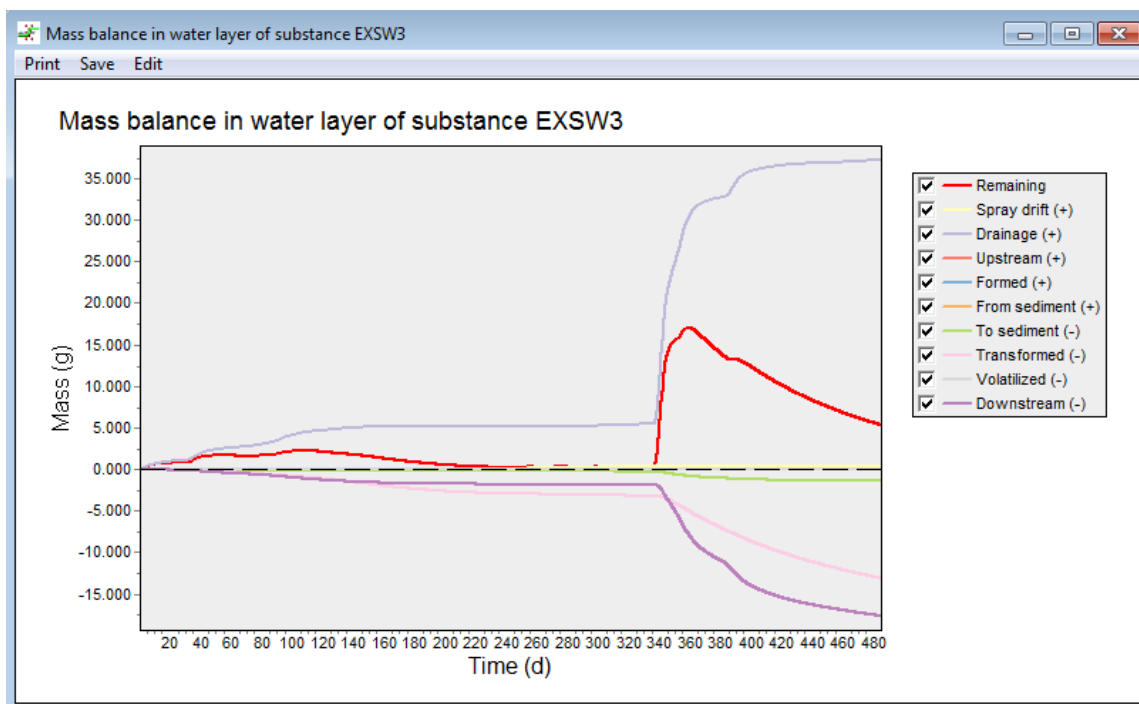


Figure 4.30 TOXSWA graph: Mass balance of pesticide in the water layer as a function of time.

The distribution of the pesticide between the compartments in the whole water body as a function of time is shown in figure 4.31. The graph is a stacked graph for the masses present in the five compartments. By selecting and deselecting the appropriate terms in the check boxes in the legends on the right hand side of the graph, the user may select which compartments are shown in the graph.

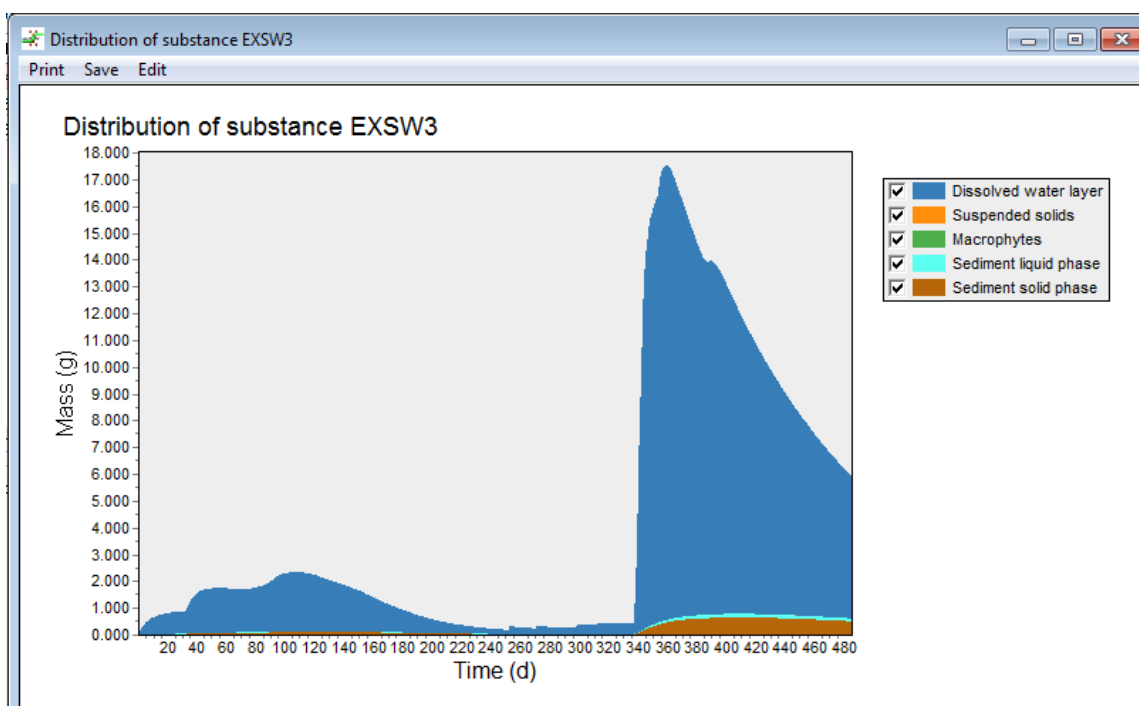


Figure 4.31 TOXSWA graph: Distribution of pesticide over water and sediment compartments as a function of time.

5 Example simulations

5.1 Water-sediment study

5.1.1 Introduction

FOCUS surface water calculations are carried out using degradation rates determined from water-sediment studies. The water-sediment study itself can be simulated with TOXSWA. The degradation rates can be fitted to the measured concentration profiles in water and in sediment using optimization tools.

In this chapter, the simulation of a water-sediment study is explained describing an example calculation. The optimization of degradation rates is, however, not described. An example of an optimization can be found in Annex 12 of FOCUS (2005), which is based on the water-sediment study also used in this chapter.

To simulate a water-sediment study with the FOCUS_TOXSWA GUI, the following steps have to be performed:

- a. creation of a project;
- b. creation of a run;
- c. definition of the location;
- d. definition of the substance;
- e. definition of the application scheme;
- f. specification of run settings.

The GUI handles simulation runs through projects. A project contains one or more runs. A run comprises a location, a substance and an application scheme. These run components can be built, bottom up, from small components, e.g. 'Sorption' for the substance component. How the run is composed with the GUI from the lowest hierarchic level up to a complete run is illustrated by the scheme in Figure 4.2 in Section 4.1.

To simulate a water-sediment study a new project needs to be created in the GUI (step a, see also Section 4.5). For the opened project, at the Runs form a run can be created using the + button (step b). On the tab 'Run Components' the user can select different components for the run (location, substance and application scheme). Run settings can be specified on the tabs 'Entries', 'Simulation Control' and 'Output Control'. Because of the bottom up approach, the sequence of the steps mentioned above should be followed. The steps c, d, e and f are explained in the Sections 5.2 to 5.5. After following these steps the simulation of the water-sediment study can be started.

5.1.2 Definition of the location

From the Runs form the TOXSWA – Locations form (Figure 4.14) can be entered to define a new scenario by pressing the ... button next to the location list box in the Runs form. A scenario location comprises a water layer, a sediment layer and a meteo station, which have to be specified in detail by the user. No specific data is necessary for the hydrology.

Before composing a new location three elements have to be created:

- water layer;
- sediment layer;
- meteo station.

How this should be done for a water-sediment study is explained in the following section.

Composing a location for the water-sediment study from the three contributing elements is described at the end of this section.

Water layer

After entering the water layers form a new water layer can be created. Figure 5.1 shows the water layers form for the example water-sediment study, where the new water layer 'C3river_ws' has been added to the list of defined water layers. The hydrology type is set to 'Constant', since there is no flow. On the 'General' tab, the length of the water layer and the bottom width of the water layer have been set to 1 m. Their values are not relevant for the simulation, because in a system with no flow, the only transport process is diffusion between the water layer and the sediment layer in the vertical direction. The water layer has to consist of 1 segment, which should be specified in 'Number of segments'. The side slope has been set to its minimum value, zero, because a test vessel has vertical walls. Setting the depth defining perimeter to zero, in combination with a side slope of 0, will set a geometry of the sediment that excludes sideways transport in sediment below the bottom of the sediment as is simulated for field water bodies (see figures 6 to 8 in Adriaanse, 1996). See also the explanation given in section 3.3.5 for the depth defining perimeter.

FOCUS_TOXSWA 4.4.2 - WaterLayer

Browse WaterLayer

Name	Hydrology type	BottomWidth	NumberOfSegments	TotalLength
D1_DITCH	WaterCourse	1	10	100
D1_STREAM	WaterCourse	1	20	100
D2_DITCH	WaterCourse	1	10	100
D2_STREAM	WaterCourse	1	20	100
D3_DITCH	WaterCourse	1	10	100
D4_STREAM	WaterCourse	1	20	100
D5_STREAM	WaterCourse	1	20	100
D6_DITCH	WaterCourse	1	10	100
R1_STREAM	WaterCourse	1	20	100
R2_STREAM	WaterCourse	1	20	100
R3_STREAM	WaterCourse	1	20	100
R4_STREAM	WaterCourse	1	20	100
Vredepeel_ditch	WaterCourse	0.5	10	100
C3river_WS	Constant	1	1	1

Edit WaterLayer

Name: C3river_WS Hydrology Type: Constant

General | Watercourse | Pond | Constant

Length water layer (m)::	1	Depth defining perimeter (m):	0
Bottom Width (m):	1	Concentration suspended solids (mg/L):	0
Number of segments:	1	Mass ratio organic matter:	0
Side slope (hor/ver):	0	Macrophytes dry weight (g/m2):	0

Close

Figure 5.1 The water layers form for the example water-sediment study, with the General tab active.

Suspended solids and macrophytes were not present in the water-sediment study, and hence the 'Concentration suspended solids', 'Mass ratio organic matter' and 'Macrophytes dry weight' are set to zero.

Since the hydrology type 'Constant' is chosen, additional parameters can be entered in the Constant tab of the water layers form (Figure 5.2). Water flow in a water-sediment study is typically zero. The

depth of the water layer can be tailored to the specific study to be simulated. In the water-sediment system used in this example the water depth was 0.06 m.

For a simulation of a water-sediment study dispersion is not relevant because the water does not flow. The entries for 'Dispersion' and 'Dispersion coefficient' are dummy values for the simulation; they are not used by TOXSWA.

Edit WaterLayer

Name: Hydrology Type:

General | Watercourse | Pond | **Constant**

Flow velocity (m/s):

Water depth (m):

Dispersion:

Dispersion coefficient (m2/d):

Close

Figure 5.2 The Constant tab of the water layers form for the example water-sediment study.

Sediment

After entering the Sediments form a new sediment object can be created. A sediment object consists of several sediment layers. Each layer is defined by a number, thickness, a building block and consists of a number of segments. Figure 5.3 shows the Sediment form for the example water-sediment study. Once a name and description have been entered for a newly defined sediment, the user can add layers in the right hand side of the form (Figure 5.3).

FOCUS_TOXSWA 4.4.2 Sediment

Browse Sediment

Name	Description
FOCUS	Focus Sediment
FOCUS_highKoc	Focus_highKoc Sediment
Vredepeel	Vredepeel sediment
C3river_WS-sediment	Sediment layer for water-sediment exan

Edit Sediment

Name:

Description:

Sediment properties:

Browse Sediment layer

Sub layer no.	Building block	Thickness	Number of seg
<not available>	<not available>	<not available>	<not available>

Edit Sediment layer

Sub layer no.:

Sediment Building Block code:

Thickness of sub layer (m):

No of segments:

Close

Figure 5.3 The sediment form for the example water-sediment study.

Because of the bottom up approach in the GUI, Building Blocks needed for the definition of the sediment layers should be defined first. The Building blocks form can be entered by pressing the ... button next to the 'Sediment Building Block Code' and is shown in Figure 5.4. To be able to add building blocks (see footnote 3 in section 4.8.2) an existing sediment object must be selected before entering the building blocks form.

Browse buildingblocks

Name	BulkDensity	Porosity	Tortuosity
FOCUS-SB1	800	0.6	0.6
Vredepeel-SB1	80	0.82	0.82
Vredepeel-SB2	220	0.77	0.77
Vredepeel-SB3	670	0.77	0.77
Vredepeel-SB4	1500	0.36	0.28
C3river_WS	1536	0.417	0.364

Edit buildingblocks

Name: C3river_WS

Dry bulk density (kg/m3): 1536

Porosity: 0.417

Tortuosity: 0.364

Mass ratio of organic matter (kg/kg): 0.016

Dispersion length (m): 0.05

Close

Figure 5.4 The sediment building blocks form for the example water-sediment study.

The composition of the sediment in the example water-sediment study was 3.9% clay, 6.0% silt, 90.1% sand and 0.9% organic carbon on mass basis. Because the sediment layer is assumed to be homogeneous, only one sediment building block is necessary. The characteristics of the building block are presented in Table 5.1. The dry bulk density of the sediment is not known. Therefore, it has been calculated from the texture data using Eq. 5.3 in Beltman *et al.* (2006). The median particle size of the sand was estimated as 160 μm , based on the particle size class of 105 – 210 μm indicated for low-loam sandy soils by Wösten *et al.* (2001). The porosity has been calculated using Eqs 5.4 and 5.5 (Beltman *et al.*, 2006). The tortuosity has been calculated with Eq. 5.6 (Beltman *et al.*, 2006). The organic carbon of the sediment of 0.9% has been converted into organic matter content by multiplying by 1.724 according to FOCUS (2003).

Table 5.1

Parameter values for the sediment in the example water-sediment study

Parameter	Value
Thickness of layer (m)	0.025
Dry bulk density (kg m ⁻³)	1536
Porosity (-)	0.417
Tortuosity (-)	0.364
Mass ratio of organic matter (kg kg ⁻¹)	0.016

Note that the dry bulk density, porosity and tortuosity differ from the values given in Annex 12 of FOCUS (2005), because slightly different equations have been used, i.e. additional soil data have been used to derive Eq. (5.3). (see Beltman et al., 2006).

Because there is no flow in sediment in the water-sediment study, there is also no dispersion, and the value of 'Dispersion length' is a dummy value for the simulation.

Next the sediment object can be defined by creating new layers (Figure 5.5). Each layer contains a building block and consists of a specified number of segments with the same thickness. Note that you need to specify the entire thickness of the layer. Therefore, a layer of 0.05 m needs 5 segments to get a thickness of 0.01 m per segment. It is advised to use thin segments of about 0.001 m in the top 0.005 m (0.5 cm) of the sediment. For compounds with high K_{oc} values, the thickness should be even smaller (see Section 4.4.3). Because the K_{oc} of the example substance is 76 000 L/kg, thin segments have been used. For simplicity, the same segmentation as for the FOCUS-highK_{oc} sediment is used, except for layer 8, where 3 segments of 0.005 m have been defined instead of 2 segments of 0.005 m. The total thickness of the sediment in the example water-sediment study was 0.025 m.

For 'Sediment properties' the option 'Input' is used, because all properties were entered in the Building blocks form.

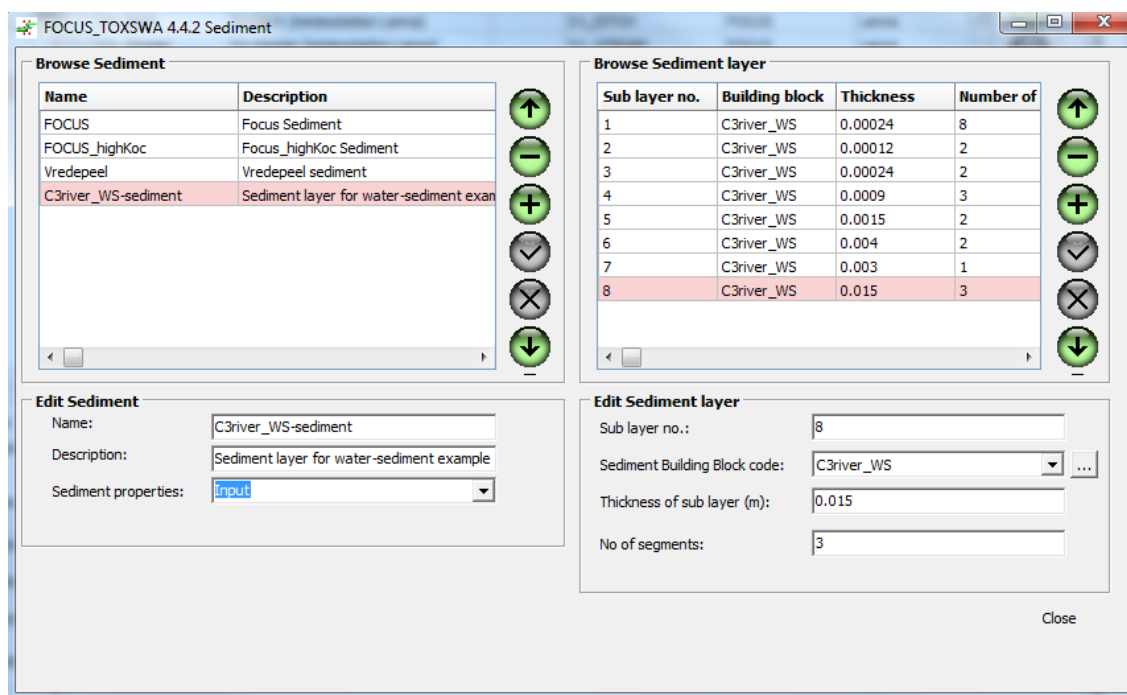


Figure 5.5 Creating a sediment from layers consisting of building blocks.

Temperature in the meteo data file

The temperature in the water-sediment system has to be specified in the meteorology file. The time span in the meteorology file has to include the period specified by the start and end dates of the simulation. The format needed for importing a meteorology file into TOXSWA is given in Figure 5.6. The file shown is used for the example water-sediment study simulation. The data in this file can be imported using the button 'Import Datafile...' on the Meteo Stations window (Figure 5.7).

```

*
* TOXSWA input file
* Filename: C:\SwashProjects\water-slib_manual\toxswa\C3-river_Water-
Sediment_study.met
* Weather station: C3-river_Water-Sediment_study
* Contents: Input data for TOXSWA concerning temperature
* Date : 11-May-2005
*
*-----
* temperature in water and sediment per month
2000 1 20.00
2000 2 20.00
2000 3 20.00
2000 4 20.00
2000 5 20.00
2000 6 20.00
2000 7 20.00
2000 8 20.00

```

Figure 5.6 Meteorology file of example water-sediment study.

Browse MeteoStations

Name	Description	StartDate	EndDate
Bologna	Bologna	01-01-1975	31-12-1994
Brimstone	Brimstone	01-01-1975	31-12-1994
La_Jailliere	La Jailliere	01-01-1975	31-12-1994
Lanna	Lanna	01-01-1980	31-12-1993
Porto	Porto	01-01-1975	31-12-1994
Roujan	Roujan	01-01-1975	31-12-1994
Skousbo	Skousbo	01-01-1975	31-12-1994
Thiva	Thiva	01-01-1977	31-12-1994
Vredepeel	Vredepeel	01-01-1975	31-12-1994
Weiherbach	Weiherbach	01-01-1975	31-12-1994

Edit MeteoStations

Caption:

Description:

Country:

Longitude (dec. degrees, East positive):

Latitude (dec degrees):

Altitude (m):

Close

Figure 5.7 Meteo stations form in TOXSWA, enabling the import of a new meteorology data file.

Note that the name of the weather station specified in the meteorology file behind '* Weather station:' should be the same as the Meteo Station Code specified in the TOXSWA GUI on the window TOXSWA – Meteo Stations (for details see Section 4.8.4). This is also explained in the pop-up box which appears after clicking the button 'Import Datafile...' (Figure 4.22).

Composition of the scenario location

When all components of the location (water layer, sediment, meteo station) have been defined, a new location can be defined by combining these elements (Figure 5.8).

The definition of the location for the water-sediment study being completed, the user can return to the Runs from of TOXSWA and select the necessary location 'C3river_Water-sediment study' on the 'Run Components' tab in order to define a Run. The other elements on the tab (Substance, Application Scheme and Initial conditions for pesticide, Figure 5.9) are discussed in sections 5.1.3, to 5.1.5.

FOCUS_TOXSWA 4.4.2 Locations

Browse Locations

Name	Description	Country	Water Layer	Sediment	Meteostation
D2_Ditch	D2 Ditch (meteostation Brimstone)		D2_DITCH	FOCUS	Brimstone
D2_Stream	D2 Stream (meteostation Brimstone)		D2_STREAM	FOCUS	Brimstone
D3_Ditch	D3 Ditch (meteo station: Vredepeel)		D3_DITCH	FOCUS	Vredepeel
D4_Pond	D4 Pond (meteo station: Skousbo)		D4_POND	FOCUS	Skousbo
D4_Stream	D4 Stream (meteo station: Skousbo)		D4_STREAM	FOCUS	Skousbo
D5_Pond	D5 Pond (meteo station: La Jailliere)		D5_POND	FOCUS	La_Jailliere
D5_Stream	D5 Stream (meteo station: La Jailliere)		D5_STREAM	FOCUS	La_Jailliere
D6_Ditch	D6 Ditch (meteo station: Thiva)		D6_DITCH	FOCUS	Thiva
R1_Pond	R1 Pond (meteo station: Weiherbach)		R1_POND	FOCUS	Weiherbach
R1_Stream	R1 Stream (meteo station: Weiherbach)		R1_STREAM	FOCUS	Weiherbach
R2_Stream	R2 Stream (meteo station: Porto)		R2_STREAM	FOCUS	Porto
R3_Stream	R3 Stream (meteo station: Bologna)		R3_STREAM	FOCUS	Bologna
R4_Stream	R4 Stream (meteo station: Roujan)		R4_STREAM	FOCUS	Roujan
C3-river_Water-sed	Example water-sediment study		C3river_WS	C3river_WS-sedime	C3-river_Water-Sedi
Vredepeel	Vredepeel	The Nethe	Vredepeel_ditch	Vredepeel	Vredepeel

Edit Locations

Name: Longitude (dec. degrees, East positive):

Description: Latitude (dec. degrees):

Country: Altitude (m):

Water Layer: ...

Sediment Layer: ...

Meteo Station: ...

Seepage flux (mm/d):

Concentration in seepage (mg/L):

Close

Figure 5.8 The TOXSWA Locations form for the example water-sediment study.

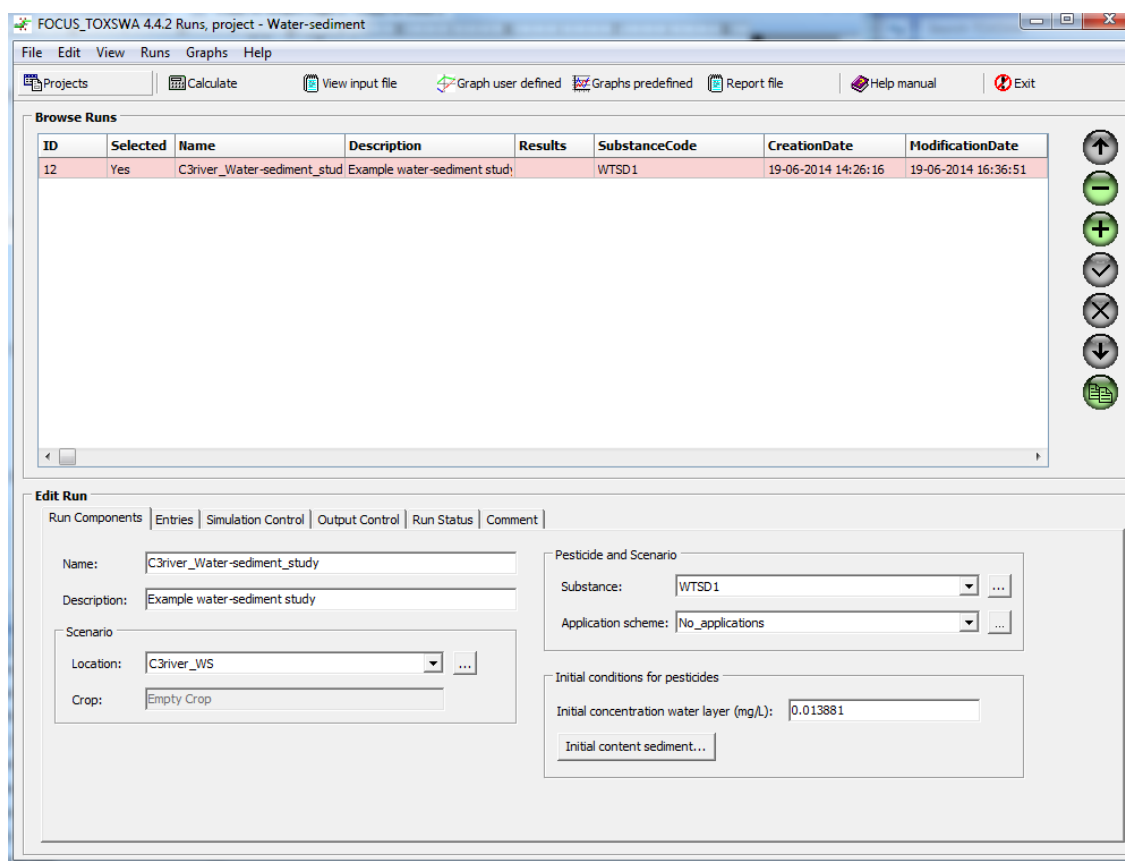


Figure 5.9 The TOXSWA Runs form for the example water-sediment study.

5.1.3 Definition of the substance


Substances are accessed from the Run components tab of the Runs form. Press the  button behind the pick list of the option field 'Substance' in the Runs form. This opens the SPIN (Substances Plug IN) program, enabling the user to add and/or edit substances (see Figure 4.22). For details about defining and editing substances from within SPIN the user is referred to the SPIN manual (van Kraalingen *et al.*, 2013)

Table 5.2 lists the parameter values of the substance of the example water-sediment study.

Table 5.2

Substance parameter values of the example water-sediment study

Parameter	Value
Molar mass (g mol ⁻¹)	418.9
Saturated vapour pressure (Pa)	1.7·10 ⁻⁷ (20 °C)
Solubility in water (mg L ⁻¹)	7.5 (25 °C)
Koc (L kg ⁻¹)	76000
Freundlich exponent, N (-)	0.9
DT50water (d-1)	0.84 (20 °C)
DT50sediment (d-1)	590.0 (20 °C)
Arrhenius activation energy (kJ mol ⁻¹)	55

5.1.4 Definition of the application scheme

From the Runs form, tab 'Run components', the Application schemes form can be accessed. An application scheme indicating that there are no applications in the water-sediment study can be added. This new application scheme can be named, e.g. 'No Loadings'. No further action is needed because Spray drift entries are not used in the simulation of the water-sediment study.

5.1.5 Specification of run settings

From the Runs form, the initial concentration and the simulation settings need to be set.

Initial concentration in the water layer

At the 'Run Components' tab, the initial concentration in the water layer needs to be specified. This should be done whilst the water-sediment scenario is selected on the tab, because the input for 'Initial concentration water layer' should correspond to the water layer of your water-sediment scenario. So, click the 'Confirm' button after entering the initial concentration in the water layer, to ensure the entry in the correct water layer.

The amount of substance added to the vessels is 42 g a.i. ha⁻¹ resulting in a concentration of 14 µg L⁻¹ in the vessels. However, this concentration does not correspond to the measurements at the start of the study, based on the measured Applied Radioactivity (AR). At zero time, 46.9%AR and 51.1%AR were found in respectively the water layer and the sediment of system 1 and 52.9%AR and 47.4%AR were found in respectively the water layer and the sediment of system 2.

Guidance for interpretation of water-sediment studies given in FOCUS (2005) indicates how to handle data for zero time: 'parent residues found in the sediment on $t = 0$ should be treated as if they were in the water column, i.e. add them to the residues in the water column'. Hence, 98%AR of the parent is attributed to the water layer of system 1 and 100.3%AR of the substance is attributed to the water layer of system 2. In order to get one number for the initial concentration for the simulation the average should be taken. The average of the two systems is 99.2%AR, corresponding to a concentration of 13.881 µg L⁻¹.

The water layer consists of one segment (Figure 5.1) so 13.881 µg L⁻¹ is allocated to this segment in the TOXSWA run. The initial concentration in the sediment is zero because it is assumed that the substance is present in the water layer only, at the start of the study.

Entries tab

At the 'Entries' tab the option for simulation of drainage or runoff should be deselected by selecting 'None' in the Type box. The choices and numerical values for the rest of the entries then become irrelevant.

Simulation

At the 'Simulation Control' tab, all default values can be used for the water-sediment study, except for the Start/Stop date entries (see also Section 4.6.6). A hypothetical start and stop date need to be given. Chosen dates and years are not important as long as the period is long enough to cover the measurement period and the time span in the meteorological file covers the start and stop dates chosen. In the example the measurements period is 105 days long. Start and stop date were chosen to be respectively 01-01-2000 and 15-04-2000, where 01-01-2000 corresponds to $t = 0$ day and 15-04-2000 to $t = 105$ day.

Output

On the 'Output Control' tab specify the thickness of the top layer. The thickness of the top layer is an output parameter for the sediment. It determines for which upper thickness of the sediment the output is given. Because the residue measured in the sediment of the water-sediment system applies to the entire sediment, it is important to get the simulated concentration of the entire sediment as output of the TOXSWA simulation. Therefore it is necessary to set the thickness of the top layer on the Output Control tab equal to the entire thickness of the sediment in the experiment (0.025 m in the example water-sediment study).

Note that the selected combination of Print method and Print time step, for the output determines whether residues can be plotted in a graph. The times specified in the output files have to match the times specified in the text files with the measurement. For example using a Time interval of output of 24 hours, the calculated concentration in the output files is given per day at 00:00 h. In the text files with the measurements, the time for each measurement is specified at 09:00. Then, the TOXSWA GUI

is not able to link the calculated concentration to the measured concentrations in the text files although the dates do correspond. Hence, it is recommended to select hourly output for water-sediment simulations. This is the default value of the GUI.

Composition of the run

On the tab 'Run Components' the components that have been defined for the water-sediment study can be selected now: the location, the substance and the application scheme (see Figure 5.9).

5.1.6 Comparison of simulated concentrations with measured concentrations

Usually the measured residues in the water layer and the sediment are expressed in % of analysed radio activity as a function of time (%AR; Table 5.3). In order to compare these figures with the concentrations simulated in water and sediment by FOCUS_TOXSWA, the residues in %AR have to be converted to concentration (g m^{-3}).

The concentration in the water layer is calculated as the initial concentration multiplied by the residue in %AR divided by 100%. For the concentration in the sediment a conversion for the difference in thickness between the water layer and the sediment (respectively 6 cm and 2.5 cm) is needed. Hence concentration in sediment = initial concentration * (%AR in sediment/100%) * (6/2.5). The results are given in Table 5.3.

When the scenario, substance, application scheme, initial concentration and simulation options of the water-sediment study have been selected, the simulation can be started by pressing the button 'Calculation'. The *.txw input file that is made by the GUI to run TOXSWA for this water-sediment study is shown in Annex 5. The concentrations in water are given in the *.out file, records with in column 3 the labels ConLiqWatLayCur, for concentration in the water layer, and ConSysSedTgt, for contents of the sediment, as a function of time (see Section 3.7 for explanation of the setup of the file. These data can then be used for optimizations and to present in graphs⁵.

Table 5.3

Residues of parent in water and in sediment of the example water-sediment study

Time (days)	Residues in water (%AR)	Residues in water (g m^{-3})	Residues in sediment (%AR)	Residues in sediment (g m^{-3})
0	46.9	0.00657	51.1	0.017170
0	52.9	0.00741	47.4	0.015926
0.25	36.1	0.00505	53.5	0.017976
0.25	41.8	0.00585	54.0	0.018144
1	35.2	0.00493	51.5	0.017304
1	32.7	0.00458	53.4	0.017942
2	15.0	0.00210	55.4	0.018614
2	16.7	0.00234	54.4	0.018278
7	1.6	0.00022	38.6	0.012970
7	1.5	0.00021	34.3	0.011525
14	2.9	0.00041	28.6	0.009610
14	N/D	N/D	25.4	0.008534
30	N/D	N/D	23.8	0.007997
30	N/D	N/D	19.5	0.006552
61	N/A	N/A	16.8	0.005645
61	N/A	N/A	12.4	0.004166
105	N/A	N/A	15.4	0.005174
105	N/A	N/A	10.5	0.003528

N/D = Not Detected, N/A = Not Analyzed

⁵ The concentrations calculated by TOXSWA can be obtained from the comprehensive *.out file of TOXSWA, e.g. by using the Sdwin tool (see Annex 7). Another simple way to obtain the data is via the GUI; plot the predefined graph for concentration in water, select Save from the menubar of the plot, select the tab Data, select the format preferred, and click the Save button. When a Text file was selected, two columns are given, the time and the concentration; these can be copied to another program to make a graph that contains both the simulated and measured data.

Water-sediment studies are used to determine transformation rates, which are used as input for FOCUS surface water calculations. The transformation rates should be determined with optimization tools. These tools minimise the differences between simulated and measured concentrations in water and in sediment. The DegT50 values found after optimization (Table 5.2) have been entered for the simulation presented in the graphs. The measured and simulated concentrations for the example water-sediment study are shown in Figure 5.10 for water and in Figure 5.11. Note that content in sediment given in table 5.3 given in $\mu\text{g/L}$ is converted to $\mu\text{g/kg}$ by dividing the concentrations in table 5.3 by the dry bulk density of the sediment of 1536 kg/m^3 (Table 5.1).

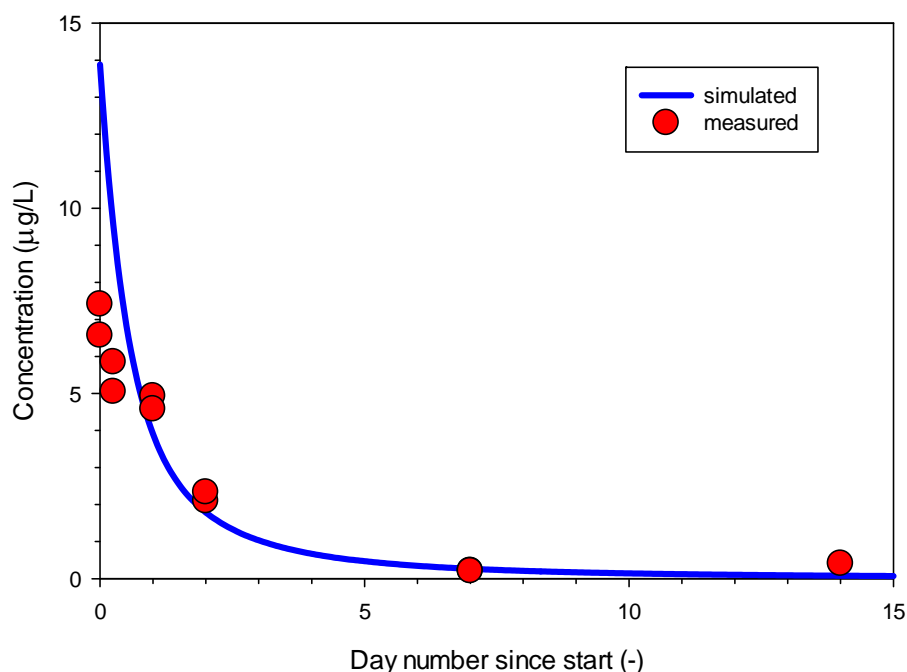


Figure 5.10 Concentration in water for the example water-sediment study; comparison of simulated and measured concentrations.

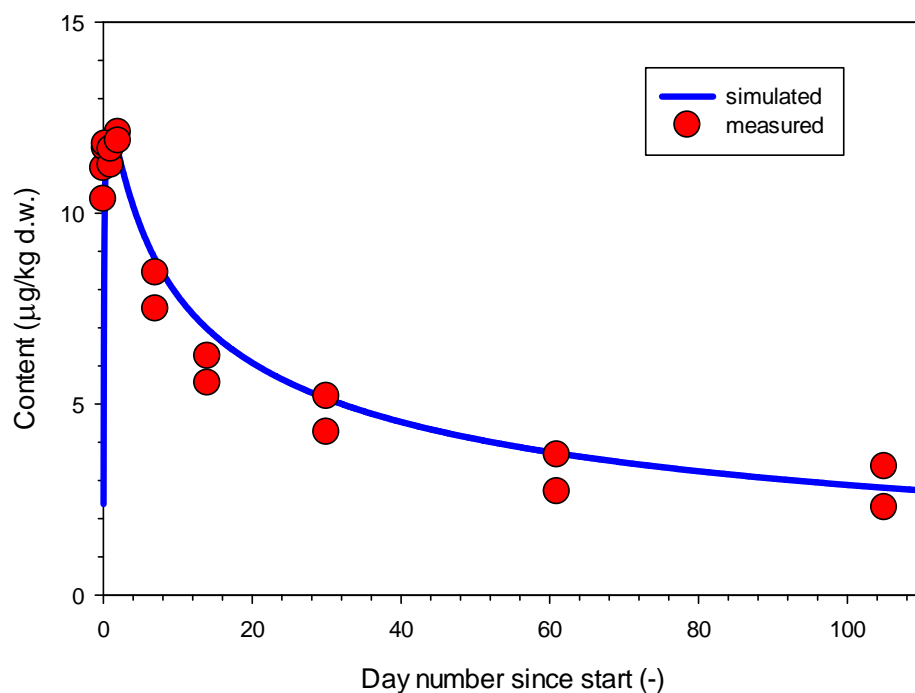


Figure 5.11 Content in sediment for the example water-sediment study; comparison of simulated and measured contents.

5.2 Multi-year run

5.2.1 Introduction

FOCUS_TOXSWA 4.4.2 has been extended with the option to simulate multiple years for FOCUS locations. FOCUS scenarios runs cover 16 months for drainage scenarios and 12 months for runoff scenarios. Sometimes simulations covering longer periods may be needed, e.g. to determine a percentile distribution of yearly exposure concentrations. In this section it is described how a multi-year run can be set up and run. The output for multi-year runs given in the summary output file is described.

SWASH can be used to setup a multi-year run, but thereafter the input for MACRO/PRZM needs to be adapted to extend the simulation period, applications etc. This is not described in this manual.

5.2.2 Specification of run settings

The steps to do a multi-year run with TOXSWA are:

- Prepare a drainage or a runoff file that covers multi-years. See the documentation of the MACRO and of the PRZM models for how to do that.
- Create a project
- Create a run
- Run Comments tab: add a location (e.g. R1pond)
- Entries tab: change settings and add a multi-year drainage or runoff file
 - Change 'Type' to 'Drainage' or 'Runoff'
 - Add 'File name' by browsing and selecting the multi-year drainage or runoff file, e.g. 100.p2t in case of 'Type' is 'Runoff'
 - Change 'Model' to 'MACRO' in case 'Type' is 'Drainage', or to 'PRZM' in case of 'Type' is 'Runoff'
 - Change 'End position' to length of water body simulated (30 m for pond, and 100 m for ditch or stream).
- Simulation Control tab: accustom the 'Begin date simulation' and 'End date simulation' to the period of the multi-year drainage or runoff file
- Run Components tab: select the substance corresponding with the substance of the soil simulation
- Run Components tab:
 - Create an application scheme: enter the number of applications that is also defined in the header of the m2t or p2t file. The application date is a dummy for simulations with drainage or runoff, so has not to be changed. Enter the application number, the dosage and the spray drift percentage for each application.
 - Select the application scheme created.

The run for a multi-year simulation is now prepared, and it can be executed by pressing 'Calculate'.

5.2.3 Output in summary file

The summary file (not the report file made by the GUI) of the run contains a section presenting the key result (i.e. annual maximum concentration) of the multi-year run. The section is shown in Figure 5.12. Note that this section is not selected in the report file that can be viewed with the GUI. Therefore locate and open the summary file by using a generic file viewer.

The table presents the maximum concentration in water in the last segment in the water layer for each simulated year, the time of occurrence in the year and the day number of the simulation. If a certain percentile value is needed from the annual maximum concentrations in the table, the concentrations can be ranked, the percentile distribution calculated, and finally the needed percentile value can be selected.

```

* TOXSWA REPORT: Exposure in Waterbody

* Table: Annual maximum exposure concentrations in water layer of substance: EXSW1
* In segment from      0.00 to      30.00 m in water body
* -----
* Year                  Concentration          Date              Daynr
*                  µg.L-1
* -----
1975                   7.986          24-Apr-1975-09h00           55
1976                   8.450          24-Apr-1976-09h00          421
1977                   8.004          24-Apr-1977-09h00           786
1978                   7.986          24-Apr-1978-09h00         1151
1979                   7.985          24-Apr-1979-09h00         1516
1980                   7.986          24-Apr-1980-09h00         1882
1981                   15.98          27-Apr-1981-14h00         2250
1982                   7.986          24-Apr-1982-09h00         2612
1983                   7.986          24-Apr-1983-09h00         2977
1984                   7.986          24-Apr-1984-09h00        3343
1985                   7.986          24-Apr-1985-09h00        3708
1986                   7.986          24-Apr-1986-09h00        4073
1987                   7.986          24-Apr-1987-09h00        4438
1988                   7.986          24-Apr-1988-09h00        4804
1989                   7.986          24-Apr-1989-09h00        5169
1990                   8.185          24-Apr-1990-09h00        5534
1991                   7.986          24-Apr-1991-09h00        5899
1992                   7.986          24-Apr-1992-09h00        6265
1993                   7.986          24-Apr-1993-09h00        6630
1994                   7.986          24-Apr-1994-09h00        6995

```

Figure 5.12 Excerpt from summary output file of TOXSWA showing PEC's for each simulated year.

Justification

This manual is an update of the manual of FOCUS_TOXSWA 2.2.1 (Beltman *et al.*, 2006). The manual was updated because the TOXSWA kernel, the Graphical User Interface and the database of FOCUS_TOXSWA have been fully redesigned and fully rebuild.

The content of this report was reviewed by Cees Vink of Alterra Wageningen UR. The project was supervised by Jennie van der Kolk (contact of WOT N&M, theme Agri-Environment) and Folkert Folkertsma (Ministry of Economic Affairs; until 1 september 2014) and Anja van Gernerden (Ministry of Economic Affairs; from 1 september 2014 onwards).

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Annex 1 FOCUS_TOXSWA input file for expert users

This annex list the extended TOXSWA input file.

```
*-----
* TOXSWA input file
* INPUT FILE for TOXSWA 3 version (f90)
*-----
* This file is intended to be used by expert users.
*
* Contact address:
* -----
* Wim Beltman
* Alterra
* PO BOX 47
* 6700 AA Wageningen
* The Netherlands
* e-mail: wim.beltman@wur.nl
*
* (c) Alterra
*
*-----
*
* Section 1: Control Section
*-----
*
01-Jan-1985      TimStart      ! Start date of simulation [01-Jan-1900 - 31-Dec-9999]
30-Apr-1986      TimEnd        ! End date of simulation [01-Jan-1900 - 31-Dec-9999]
FOCUS            CallingProgram ! Calling program in FOCUS_TOXSWA for EU authorization
4                CallingProgramVersion ! Version of calling program
4                ModelVersion    ! version number of the model
4                GUIVersion      ! version number of the GUI
2                DBVersion       ! version number of the database
Hourly           OptInp         ! Option for hourly or daily input data (Hourly, Daily)
OnLine           OptHyd         ! Hydrology simulation option (Only, OnLine, OffLine, Automatic)
OnLine           OptTem         ! Temperature simulation option (Only, OnLine, OffLine, Automatic)
600              MaxTimStpWat (s) ! Maximum calculation time step in water layer [0.001 - 3600]
600              MaxTimStpSed (s) ! Maximum calculation time step in sediment [0.001 - 3600]
600.             TimStpHyd (s)   ! Maximum calculation time step for hydrology [0.001 - 3600]
No               OptScreen      ! Option to show output on screen (Yes, No)
Calc             OptTimStp      ! Time step substance simulation options (Input, Calc)

*-----
*
* Section 2: Waterbody section
*-----
*
D4_Pond          Location      ! Name of the location
D4_POND          WaterbodyID   ! ID of the water body

* Table WaterBody
* Len            = Length (m) [0.1 - 10000]
* NumSeg         = Number of segments (-) [1 - 1000]
* WidWatSys      = Width of the bottom of water system (m) [0.1 - 100]
* SloSidWatSys   = Side slope of the water system (-) [0.001 - 2]
* DepWatDefPer   = Water depth defining perimeter for the exchange between water layer and sediment (m) [0
- lowest water depth]

table WaterBody
Len      NumSeg  WidWatSys  SloSidWatSys  DepWatDefPer
(m)      (-)     (m)        (-)          (m)
30.      1       30.        1E-005      0.01
End_table

15.       ConSus (g.m-3)      ! Concentration of suspended solids [1.0 - 100000]
0.09      CntOmSusSol (kg.kg-1) ! Mass ratio of organic matter in suspended solids [0.0 - 1.0]
0.        AmaMphWatLay (g.m-2) ! Dry weight of macrophyte biomass per m2 bottom [0.0 - 1000]

*-----
*
*
```

```

* Section 3: Hydrology: general
*-----
*

Pond                OptWaterSystemType  ! Option for selecting the water system type (Pond,
Variable            OptFloWat           ! Option for water flow (Constant, Variable)
WaterCourse)

* if: OptWaterSystemType = WaterCourse
Fischer              OptDis              ! Options are 'Fischer' and 'Input'

* if: OptDis = Input
0.                   CofDisPhsInp (m2.d-1) ! Dispersion coefficient [0. - 100000]
*-----
*

* Section 3a: Constant water flow
*-----
*

* if: OptFloWat = Constant
1.                   DepWat (m)
0.                   VelWatFlwBas (m.d-1)
*-----
*

* Section 3b: Variable water flow: pond
*-----
*

* if: OptFloWat = Variable and OptWaterSystemType = Pond
0.45                 AreaSurPndInp (ha)    ! Size of area surrounding the pond [0.0 - 50.0]

* if: CallingProgram = FOCUS
3.189                QBasPndInp (m3.d-1)   ! Base flow, i.e. inflow into pond [0.001 - 50.0]
1.                   HgtCrePnd (m)         ! Height of the weir crest [0.1 - 5.0]
0.5                  WidCrePnd (m)         ! Width of the weir crest [0.01 - 10]

* if: Opt = Runoff
0.06                 AreaErsSurPndInp (ha) ! Size of the eroding area around the pond [0.0 - 50.0]
*-----
*

* Section 3c: Variable water flow: watercourse
*-----
*

* if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
*representative channel
0.                   SloBotRepCha (-)      ! Slope bottom representative channel [0.0 - 0.01]
0.                   HgtCreRepCha (m)      ! Height of the weir crest [0.1 - 5.0]
0.                   WidCreRepCha (m)      ! Width of the weir crest [0.01 - 10]

0.                   LenRepCha (m)         ! Length representative channel [10.0 - 2000]
0.                   WidBotRepCha (m)      ! Width bottom representative channel [0.1 - 10]
0.                   SloSidRepCha (-)      ! Side slope of the representative channel [0.0 - 10]

0.                   CofRghRef (-)         ! Value of the Manning coefficient for bottom roughness [1.0-100]
0.                   CofVelHea (-)         ! Energy coefficient resulting from the non-uniform distribution
                                         of flow velocities [1.1 - 1.5]

* if: CallingProgram = NL or FOCUS
0.                   AreaUpsWatCrsInp (ha) ! Size of the area upstream the representative channel
                                         [0.0 - 10000]
0.                   QBasWatCrsInp (m3.d-1)! Minimal flow into watercourse [0.0 10000]

0.                   AreaUpStrRepCha (ha)  ! Size of the area upstream the representative channel
                                         [0.0 - 10000]
0.                   QBasRepCha (m3.d-1)   ! Minimal flow into watercourse [0.0 - 10000]
*-----
*

* Section 4: Sediment section
*-----
*

FOCUS                SedimentTypeID      ! Name of sediment type

* table SedimentProfile
* ThiHor = thickness of horizon [0.0001 - ]
* NumLay = number of layers in horizon [1,]

table SedimentProfile
ThiHor    NumLay
(m)
0.004     4
0.006     3
0.01      2
0.03      3
0.02      1
0.03      1
end_table

Input          OptSedProperties      ! Option sediment properties [Input, Calc]

* table specifying SedimentProperties for each horizon:
* Nr           = number horizon [1,]
* Rho          = bulk density [100 - 2000]

```

```

* CntOm      = organic matter mass content [0.1 - 1.0]
* ThetaSat   = saturated water content [0.1 - 0.95]
* CofDifRel  = relative diffusion coefficient [0.0 - 1.0]

table horizon SedimentProperties
Nr      Rho      CntOm      ThetaSat  CofDifRel
        (kg.m-3) (kg.kg-1) (m3.m-3)  (-)
1        800.      0.09      0.6        0.6
2        800.      0.09      0.6        0.6
3        800.      0.09      0.6        0.6
4        800.      0.09      0.6        0.6
5        800.      0.09      0.6        0.6
6        800.      0.09      0.6        0.6
end_table

0.      FlwWatSpg (m3.m-2.d-1)

* If: FlwWatSpg not zero
* table horizon DispersionLength
* Nr      = Horizon number []
* LenDisSedLiq = Dispersion length of solute in liquid phase [0.05 - 1.0]

table horizon DispersionLength
Nr      LenDisSedLiq
        (m)
1        0.015
2        0.015
3        0.015
4        0.015
5        0.015
6        0.015
end_table

* If: OptLoa = PRZM
0.01      ThiLayErs (m)! Thickness of sediment layer to which eroded soil is added [0.0001- ]
*-----
*
* Section 5: Weather section
*-----
*

Skousbo      MeteoStation  ! Name of the *.met file with meteo data

Monthly      OptMetInp      ! Option for hourly or daily input data (Hourly, Daily, Monthly)

*-----
*
* Section 6: Compound section
*-----
*

EXSW2      SubstanceName  ! Name of parent substance [1 - 6 characters]

table compounds      ! List of substances [1 - 6 characters]
EXSW2
end_table

* Table parent-daughter relationships transformation in water (FraPrtDauWat):
* Column 1: fraction formed from parent into daughter
* Column 2: name of parent
* Column 3: name of daughter

table FraPrtDauWat (mol.mol-1)
end_table

* Table parent-daughter relationships transformation in sediment (FraPrtDauSed):
* Column 1: fraction formed from parent into daughter
* Column 2: name of parent
* Column 3: name of daughter

Table FraPrtDauSed (mol.mol-1)
end_table

* Substance properties for each substance given in table compounds
* Substance code is extension of parameter name
*----- Parent: EXSW2 -----

300.      MolMas_EXSW2 (g.mol-1)  ! Molar mass of parent substance [10.0 - 10000]

100.      DT50WatRef_EXSW2 (d)    ! Half-life transformation in water [0.1 - 100000]
20.      TemRefTraWat_EXSW2 (C)  ! Temperature at which half-life was measured [5.0 - 30]
65.4     MolEntTraWat_EXSW2 (kJ.mol-1) ! Molar activation enthalpy of transformation in
                                         water [0.0 - 200]

300.      DT50SedRef_EXSW2 (d)    ! Half-life transformation in sediment [0.1 - 100000]
20.      TemRefTraSed_EXSW2 (C)  ! Temperature at which half-life was measured [5.0 - 30]
65.4     MolEntTraSed_EXSW2 (kJ.mol-1) ! Molar activation enthalpy of transformation in
                                         sediment [0.0 - 200]

58.      KomSed_EXSW2 (L.kg-1)   ! Coefficient of equilibrium sorption in sediment
                                         [0.0 - 10000000]
1.      ConLiqRefSed_EXSW2 (mg.L-1) ! Reference concentration in liquid phase in
                                         sediment [0.001 - 100]
1.      ExpFreSed_EXSW2 (-)      ! Freundlich exponent in sediment [0.1 - 2]

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58.      KomSusSol_EXSW2 (L.kg-1) ! Coefficient of equilibrium sorption suspended
      solids [0.0 - 10000000]
1.      ConLiqRefSusSol_EXSW2 (mg.L-1) ! Reference concentration in liquid phase
      suspended solids [0.001 - 100]
1.      ExpFreSusSol_EXSW2 (-) ! Freundlich exponent suspended solids [0.1 - 2]
0.      CofSorMph_EXSW2 (L.kg-1) ! Coefficient for linear sorption on macrophytes
      [0.0 - 20000]
1.E-7    PreVapRef_EXSW2 (Pa) ! Saturated vapour pressure [0.0 - 200000]
20.      TemRefVap_EXSW2 (C) ! Temperature of reference at which the saturated vapour
      pressure was measured [0.0 - 40]
95.      MolEntVap_EXSW2 (kJ.mol-1) ! Molar enthalpy of the vaporization process
      [-200 - 200]

1.      SlbWatRef_EXSW2 (mg.L-1) ! Water solubility [0.001 - 1000000]
20.      TemRefSlb_EXSW2 (C) ! Temperature of reference at which the water solubility
      was measured [0.0 - 40]
27.      MolEntSlb_EXSW2 (kJ.mol-1) ! Molar enthalpy of the dissolution [-200 - 200]
4.3E-5   CofDifWatRef_EXSW2 (m2.d-1) ! Reference diffusion coefficient in water[0.0-200]

*-----
*
* Section 7: Management section
*-----
*

* Loading options (OptLoa):
* DriftOnly = spray drift only entry route
* PEARL      = drainage calculated by PEARL
* MACRO      = drainage calculated by MACRO
* PRZM       = runoff and erosion calculated by PRZM
* GEM        = point source calculated by GEM

MACRO      OptLoa      ! Loading options (DriftOnly, PEARL, MACRO, PRZM, GEM)

FOCUS_EXAMPLE ApplicationScheme ! Name of the application scheme

* Table loadings
* Column 1: Date of application, relevant if OptLoa = DriftOnly, otherwise the date is a dummy values
* Column 2: Type of loading (-)
* Column 3: Drift deposition (mg.m-2) []
* Column 4: Start of stretch of watercourse loaded by all loading types (m) []
* Column 5: End of stretch of watercourse loaded by all loading types (m) []

table Loadings
30-Dec-1899 drift      0.154      0.      30.
30-Dec-1899 drift      0.1155     0.      30.
30-Dec-1899 drift      0.077      0.      30.
end_table

* If: OptLoa = MACRO or OptLoa = PRZM
* Table with path+name of lateral entries files

table Soil substance files
C:\SwashProjects\Project_1\MACRO\cereals_winter\macro00001_p.m2t
end_table

* If: OptLoa = PEARL or OptLoa = MACRO
0.      WidFldDra (m)      ! Width of field contributing drainage

* If: OptLoa = PRZM
0.      WidFldRnf (m)      ! Width of field contributing runoff
0.      WidFldErs (m)      ! Width of field contributing erosion
0.      RatInfDir (-)      ! Ratio of infiltration water added to runoff water

* If: CallingProgram = FOCUS and OptWaterSystemType = WaterCourse
Yes      OptUpsInp      ! Switch for upstream catchment treated (Yes, No)
0.      RatAreaUpsApp (-) ! Ratio of upstream catchment treated [0.0 - 1]
1.      FraMetForUps (-) ! Fraction primary metabolites formed in water in upstream
      catchment
0.      ConAir (kg.m-3)    ! Concentration of the substance in air
0.      ConWatSpg (g.m-3)  ! Concentration in incoming seepage water

0.      ConSysWatIni (g.m-3)

* Table initial substance content in sediment (CntSysSedIni)
* Column 1: Depth in sediment (m)
* Column 2: Substance content (mg.kg-1)
table interpolate CntSysSedIni (mg.kg-1)
end_table

*-----
*
* Section 8: Output control
*-----
*

No      OptDelOutFiles ! Switch for removing *.out files after run (Yes, No)
FOCUS   OptReport      ! Options for report type (DutchRegistration, FOCUS)
Yes      ExposureReport ! Exposure report (Yes, No)
No      PercentileReport ! Percentile report (Yes, No)
DaysFromSta DateFormat ! Date format (DaysFromSta, DaysFrom1900, Years)
e14.6    RealFormat     ! Number format of the reals

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```

0.05          ThiLayTgt (m)      ! Thickness of the target layer
Hour          OptDelTimPrn      ! Option to set output time step (Hour, Day, Decade, Month, Year,
Automatic, Other)
1            DelTimPrn (d)      ! Output time step [0.0 - length simulation period]
No          PrintCumulatives    ! Specify whether fluxes should be cumulated over the entire
simulation period (Yes, No)

* table HorizontalProfiles: dates are given for which detailed output is wished
* Column 1: dates

table HorizontalProfiles
end_table

* Table output depths (OutputDepths): indicate for which depths the output is selected
* Column 1: Depth

table OutputDepths (m)
0.005
0.045
0.095
end_table

All OptOutputDistances ! Switch output distances (None, All, Table)

* Table output distances (OutputDistances): indicate for which distance the output is selected
* Column 1: Distance

table OutputDistances (m)
15.
30.
10.
end_table

No          print_VelWatFlw      ! Flow velocity (m/h) [Yes, No]
Yes         print_QBou          ! Discharge (m3/h) [Yes, No]
No          print_VvrLiqDra      ! Drain flow (m/h) [Yes, No]
No          print_VvrLiqRnf      ! Runoff flow [Yes, No]
No          print_FlmDra         ! Drain substance flux [Yes, No]
No          print_FlmRnf         ! Runoff substance flux [Yes, No]
No          print_FlmErs         ! Erosion substance flux [Yes, No]
Yes         print_ConLiqWatLay   ! Concentration in water, hour average (g/m3) [Yes,
No          print_ConSysWatLay   ! Total concentration in water (g/m3) [Yes, No]
No          print_CntSorMph       ! Content sorbed to macrophytes [Yes, No]
No          print_CntSorSusSol    ! Content sorbed suspended solids [Yes, No]
No          print_ConSysSed       ! Total content in sediment [Yes, No]
No          print_ConLiqSed       ! Concentration in pore water sediment (g/m3) [Yes,
No          print_CntSorSed       ! Content sorbed to sediment [Yes, No]
No          print_DepWat         ! Water depth (m) [Yes, No]
No          print_DepWatRepCha    ! Water depth representative channel [Yes, No]
Yes         print_CntSedTgt       ! Total content in target layer sediment [Yes, No]
No          print_ConLiqSedTgt    ! Concentration in pore water in target layer sediment
No          print_CntSorSedTgt    ! Content sorbed in target layer sediment [Yes, No]
Yes         print_ConLiqWatLayCur ! Concentration in water, at end hour (g/m3) [Yes, No]
Yes         print_AmaWatLay       ! Mass in water layer [Yes, No]
Yes         print_AmaLiqWatLay    ! Mass in liquid phase in water layer [Yes, No]
Yes         print_AmaSorSusSol    ! Mass sorbed to suspended solids in water layer [Yes,
Yes         print_AmaSorMph       ! Mass sorbed to macrophytes in water layer [Yes, No]
Yes         print_AmaSed         ! Mass in sediment layer [Yes, No]
Yes         print_AmaLiqSed       ! Mass in liquid phase in sediment layer [Yes, No]
Yes         print_AmaSorSed       ! Mass sorbed in sediment layer [Yes, No]
Yes         print_AmaTraWatLay    ! Mass transformed in water layer [Yes, No]
Yes         print_AmaForWatLay    ! Mass formed in water layer [Yes, No]
Yes         print_AmaVolWatLay    ! Mass volatilised in water layer [Yes, No]
Yes         print_AmaSedInWatLay  ! Mass penetrated into sediment from water layer [Yes,
Yes         print_AmaSedOutWatLay ! Mass transferred from sediment into water layer [Yes,
Yes         print_AmaDwnWatLay    ! Mass flowed across downstream boundary out of water
layer [Yes, No]
Yes         print_AmaUpsWatLay    ! Mass flowed across upstream boundary into water
layer [Yes, No]
Yes         print_AmaDrfWatLay    ! Mass entered water layer by spray drift [Yes, No]
Yes         print_AmaAtmDepWatLay ! Mass entered water layer by atmospheric deposition
Yes         print_AmaDraWatLay    ! Mass entered water layer by drainage [Yes, No]
Yes         print_AmaRnoWatLay    ! Mass entered water layer by runoff [Yes, No]
Yes         print_AmaTraSed       ! Mass transformed in sediment layer [Yes, No]
Yes         print_AmaForSed       ! Mass formed in sediment layer [Yes, No]
Yes         print_AmaWatLayInSed  ! Mass transferred into water layer from sediment
Yes         print_AmaWatLayOutSed ! Mass transferred from water layer into sediment layer
Yes         print_AmaDwnSed       ! Mass leaving sediment layer across lower boundary
Yes         print_AmaErsSed       ! Mass entering sediment layer by erosion [Yes, No]
No          print_VolErrWatLay    ! Volume error in waterbody [Yes, No]
No          print_AmaErrWatLay    ! Mass error in mass balance of the waterlayer [Yes,
No          print_ConLiqWatLayNLAv ! Concentration in water, average in evaluation
stretch [Yes, No]

*-----
* End of TOXSWA input file
*-----

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Annex 2 Technical description of the TOXSWA input file

ID	Units						Limits on value	Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth			
Section 1									
TimStart	-	S	1	N	N	N	01-Jan-1900 31-Dec-9999	Starting time of simulation	
TimEnd	-	S	1	N	N	N	01-Jan-1900 31-Dec-9999	End time of simulation	
CallingProgram	-	S	1	N	N	N	FOCUS	Version of CallingProgram	
CallingProgramVersion	-	S	1	N	N	N	integer.integer.integer	Version numbers (model.GUI.database)	
OptInp	-	S	1	N	N	N	Hourly,Daily	Option for hourly or daily input data	
OptDelTimPrn	-	S	1	N	N	N	Hour,Day,Decade,Month,Year,Automatic,Other	Option to set output time step	
DelTimPrn	d	S	1	N	N	N	1, length simulation period	Output time step	If: OptDelTimPrn = Other
PrintCumulatives	-	S	1	N	N	N	Yes,No	Specify whether fluxes should be cumulated over the entire simulation period	
OptHyd	-	S	1	N	N	N	Only,OnLine,OffLine,Automatic	Hydrology simulation option	
OptTem	-	S	1	N	N	N	Only,OnLine,OffLine,Automatic	Temperature simulation option	
OptTimStp	-	S	1	N	N	N	Input,Calc	Time step substance simulation options	
MaxTimStpWat	s	S	1	N	N	N	0.001 3600	Maximum calculation time step in water layer	If: OptTimStp = Input
MaxTimStpSed	s	S	1	N	N	N	0.001 3600	Maximum calculation time step in sediment layer	If: OptTimStp = Input
TimStpHyd	s	S	1	N	N	N	0.001 3600	Calculation time step for hydrology	
OptScreen	-	S	1	N	N	N	Yes,No	Option to show output on screen	
IOMode	-	S	1	N	N	N	IOMode_std,IOMode_Full	Screen output control	
Section 2									
Location	-	S	1	N	N	N	1-250 characters	Name of the location	
WaterbodyID	-	S	1	N	N	N	1-250 characters	ID of the water body	
table Waterbody: column 1 Len	m	S	1	N	N	N	0.05 10000	Length	
table Waterbody: column 2 NumSeg	-	S	1	N	N	N	1 -	Number of segments	Maximally 1000 segments
table Waterbody: column 3 WidWatSys	m	S	1	N	N	N	0.05 100	Width of the bottom of water system	
table Waterbody: column 4 SloSidWatSys	-	S	1	N	N	N	0.0 10	Side slope of the water system	
table Waterbody: column 5 DepWatDefPer	m	S	1	N	N	N	0.0 lowest water depth	Water depth defining perimeter for exchange between water layer and sediment	

ID	Units						Limits on value	Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth			
ConSus	g.m ⁻³	S	1	N	N	N	0.0 100000	Concentration of suspended solids	
CntOmSusSol	g.g ⁻¹	S	1	N	N	N	0.0 1	Mass ratio of organic matter in suspended solids	
AmaMphWatLay	g.m ⁻²	S	1	N	N	N	0.0 1000	Dry weight of macrophyte biomass per m2 bottom	
Section 3									
OptWaterSystemType	-	S	1	N	N	N	Pond, WaterCourse,Constant	Option for selecting the water system type	
OptFloWat	-	S	1	N	N	N	Constant, Variable	Option for water flow	
OptDis	-	S	1	N	N	N	Fischer,Input	Option for selecting dispersion method	if: OptWaterSystemType = WaterCourse
CofDisPhsInp	m ² .d ⁻¹	S	1	N	N	N	0.0 1000000	Dispersion coefficient	if: OptWaterSystemType = WaterCourse and OptDis = Input
DepWat	m	S	1	N	N	N	0.001 10	Water depth	if: OptFloWat = Constant
VelWatFlwBas	m.d ⁻¹	S	1	N	N	N	-100000.0 100000.0	Flow velocity	if: OptFloWat = Constant
AreaSurPndInp	ha	S	1	N	N	N	0.0 100	Size of area surrounding the pond	if: OptFloWat = Variable and OptWaterSystemType = Pond
QBasPndInp	m ³ .d ⁻¹	S	1	N	N	N	0.0 50	Base flow, i.e. inflow into pond	if: OptFloWat = Variable and OptWaterSystemType = Pond
HgtCrePnd	m	S	1	N	N	N	0.1 5	Height of the weir crest	if: OptFloWat = Variable and OptWaterSystemType = Pond
WidCrePnd	m	S	1	N	N	N	0.01 10	Width of the weir crest	if: OptFloWat = Variable and OptWaterSystemType = Pond
AreaErsSurPndInp	ha	S	1	N	N	N	0.0 100	Size of the eroding area around the pond	if: OptFloWat = Variable and OptWaterSystemType = Pond and Opt = Runoff
AreaUpsWatCrSInp	ha	S	1	N	N	N	0.0 10000	Area of upstream catchment	if: OptFloWat = Variable and OptWaterSystemType = WaterCourse

ID	Units						Limits on value	Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth			
QBasWatCrsInp	m ³ .d ⁻¹	S	1	N	N	N	0.0 10000	Base flow from upstream catchment	if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
AreaUpsStrRepCha	ha	S	1	N	N	N	0.0 10000	Area of upstream catchment	if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
QBasRepCha	m ³ .d ⁻¹	S	1	N	N	N	0.0 10000	Base flow from upstream catchment	if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
SloBotRepCha	-	S	1	N	N	N	0.0 0.01	Slope bottom representative channel	if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
HgtCreRepCha	m	S	1	N	N	N	0.01 5	Height of the weir crest	if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
WidCreRepCha	m	S	1	N	N	N	0.01 10	Width of the weir crest	if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
LenRepCha	m	S	1	N	N	N	10.0 2000	Length representative channel	if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
WidBotRepCha	m	S	1	N	N	N	0.1 10	Width bottom representative channel	if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
SloSidRepCha	-	S	1	N	N	N	0.0 10	Side slope of the representative channel	if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
CofRghRef	-	S	1	N	N	N	1.0 100	Value Manning coefficient for bottom roughness at 1 m water depth in water body	if: OptFloWat = Variable and OptWaterSystemType = WaterCourse

ID	Units	Limits on value					Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth		
CofVelHea	-	S	1	N	N	N	1.1-1.5	Energy coefficient due to non-uniform distribution of flow velocities in cross section if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
Section 4								
SedimentTypeID	-	S	1	N	N	N	1-250 characters	Name of sediment type
table Sedimentprofile: column 1 ThiHor	m	A	no	N	N	N	0.0001 -	Thickness of horizon
table Sedimentprofile: column 2 NumLay	-	A	no	N	N	N	1 -	Number of layers in horizon Maximally 100 layers
OptSedProperties	-	S	1	N	N	N	Input,Calc	Option sediment properties
table horizon SedimentProperties: column 1 Nr	-	A	no	N	N	N	1 -	Number horizon Maximally 100 horizons
table horizon SedimentProperties: column 2 Rho	kg.m ⁻³	A	no	N	N	N	10 3000	Bulk density
table horizon SedimentProperties: column 3 CntOm	kg.kg ⁻¹	A	no	N	N	N	0.0 1	Organic matter mass content
table horizon SedimentProperties: column 4 ThetaSat	m ³ .m ⁻³	A	no	N	N	N	0.001 0.999	Saturated water content
table horizon SedimentProperties: column 5 CofDifRel	-	A	no	N	N	N	0.0 1	Relative diffusion coefficient
table horizon DispersionLength: column 1 Nr	-	A	no	N	N	N	1 -	Number horizon if: FlwWatSpg not zero Maximally 100 horizons
table horizon DispersionLength: column 2 LenDisSedLiq	m	A	no	N	N	N	0.01 1	Dispersion length of solute in liquid phase if: FlwWatSpg not zero
FlwWatSpg	m ³ .m ⁻² .d ⁻¹	S	1	N	N	N	0.0 0.01	Rate of percolation through the sediment

ID	Units						Limits on value	Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth			
Section 5									
MeteoStation	-	S	1	N	N	N	1-250 characters	Name of the *.met file with meteo data	
OptMetInp	-	S	1	N	N	N	Hourly,Daily,Monthly	Option for hourly or daily input data	
Section 6									
SubstanceName	-	S	1	Y	N	N	1-6 characters	Name of parent substance	
table compounds: column 1	-	A	no	Y	N	N	1-6 characters	Names of all substances	Parent must be in list maximally 20 substances
table FraPrtDauWat : column 1	-	A	no	Y	N	N	0.0 -	Fraction formed from parent into daughter	
table FraPrtDauWat : column 2	-	A	no	Y	N	N	Name substance	Name of parent	
table FraPrtDauWat: column 3	-	A	no	Y	N	N	Name substance	Name of daughter	
table FraPrtDauSed : column 1	-	A	no	Y	N	N	0.0 -	Fraction formed from parent into daughter	
table FraPrtDauSed : column 2	-	A	no	Y	N	N	Name substance	Name of parent	
table FraPrtDauSed: column 3	-	A	no	Y	N	N	Name substance	Name of daughter	
For each substance									SubstanceName [name] coupled to each substance property
MolMas_[name]	g.mol ⁻¹	S	1	Y	N	N	10.0 10000	Molar mass	
DT50WatRef_[name]	d	S	1	Y	N	N	0.1 100000	Half-life transformation in water	
TemRefTraWat_[name]	C	S	1	Y	N	N	5.0 30	Temperature at which half-life was measured	
MolEntTraWat_[name]	kJ.mol ⁻¹	S	1	Y	N	N	0.0 200	Molar activation enthalpy of transformation	
DT50SedRef_[name]	d	S	1	Y	N	N	0.1 100000	Half-life transformation in sediment	
TemRefTraSed_[name]	C	S	1	Y	N	N	5.0 30	Temperature at which half-life was measured	
MolEntTraSed_[name]	kJ.mol ⁻¹	S	1	Y	N	N	0.0 200	Molar activation enthalpy of transformation	
KomSed_[name]	L.kg ⁻¹	S	1	Y	N	N	0.0 10000000	Coefficient of equilibrium sorption in sediment	
ConLiqRefSed_[name]	mg.L ⁻¹	S	1	Y	N	N	0.0 10000000	Reference concentration in liquid phase in sediment	

ID	Units						Limits on value	Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth			
ExpFreSed_[name]	-	S	1	Y	N	N	0.1 1.5	Freundlich exponent in sediment	
KomSusSol_[name]	L.kg ⁻¹	S	1	Y	N	N	0.0 10000000	Coefficient of equilibrium sorption suspended solids	
ConLiqRefSusSol_[name]	mg.L ⁻¹	S	1	Y	N	N	0.001 100	Reference concentration in liquid phase suspended solids	
ExpFreSusSol_[name]	-	S	1	Y	N	N	0.1 1.5	Freundlich exponent suspended solids	
CofSorMph_[name]	L.kg ⁻¹	S	1	Y	N	N	0.0 10000000	Coefficient for linear sorption on macrophytes	
PreVapRef_[name]	Pa	S	1	Y	N	N	0.0 200000	Saturated vapour pressure of substance	
TemRefVap_[name]	C	S	1	Y	N	N	0.0 40	Temperature of reference at which the saturated vapour pressure was measured	
MolEntVap_[name]	kJ.mol ⁻¹	S	1	Y	N	N	-200 200	Molar enthalpy of the vaporization process	
SibWatRef_[name]	mg.L ⁻¹	S	1	Y	N	N	0.001 1000000	Water solubility of substance	
TemRefSib_[name]	C	S	1	Y	N	N	0.0 40	Temperature of reference at which the water solubility was measured	
MolEntSib_[name]	kJ.mol ⁻¹	S	1	Y	N	N	-200.0 200.0	Molar enthalpy of the dissolution	
CofDifWatRef_[name]	m ² .d ⁻¹	S	1	Y	N	N	0.0 200.0E-5	Reference diffusion coefficient in water	
Section 7									
OptLoa	-	S	1	N	N	N	DriftOnly,PEARL,MACRO,PRZM,GE M	Loading options	
ApplicationScheme	-	S	1	N	N	N	1-250 characters	Name of the applicaton scheme	
table Loadings: column 1	-	A	no	N	N	N	simulation period	Date of application, relevant if OptLoa = 'DriftOnly', otherwise the date is a dummy values	maximally 1000 values
table Loadings: column 2	-	A	no	N	N	N	-	Type of loading	maximally 1000 values
table Loadings: column 3	mg.m ⁻²	A	no	N	N	N	0. -	Drift deposition	maximally 1000 values
table Loadings: column 4	m	A	no	N	N	N	0.0 10000	Start of stretch of watercourse loaded by all loading types	maximally 1000 values
table Loadings: column 5	m	A	no	N	N	N	0.0 10000	End of stretch of watercourse loaded by all loading types	maximally 1000 values
table Soil Substances: column 1	-	A	3	Y	N	N	1-250 characters	Table lateral entries file of soil substance (path+name)	if: OptLoa = MACRO or OptLoa = PRZM

ID	Units						Limits on value	Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth			
WidFldDra	m	S	1	N	N	N	0.0 1000	Width of field contributing drainage	if: OptLoa = MACRO
WidFldRnf	m	S	1	N	N	N	0.0 1000	Width of field contributing runoff	if: OptLoa = PRZM
WidFldErs	m	S	1	N	N	N	0.0 1000	Width of field contributing erosion	if: OptLoa = PRZM
RatInfDir	-	S	1	N	N	N	0.0 1	Ratio of infiltraton water added to runoff water	if: OptLoa = PRZM
ThiLayErs	m	S	1	N	N	N	0.00001 1	Thickness of layer to which erosion mass is added	if: OptLoa = PRZM
OptUpsInp	-	S	1	N	N	N	Yes,No	Switch for upstream catchment treated	
RatAreaUpsApp	-	S	1	N	N	N	0.0 1.0	Ratio of upstream catchment treated	
FraMetForUps	-	S	1	N	N	N	0.0 1	Fraction primary metabolite formed in water in upstream catchment	
ConSysWatLayIni	mg.L ⁻¹	S	1	N	N	N	0.0 -	Initial total concentration in water layer	
ConAir	g.m ⁻³	S	1	N	N	N	0.0 -	Concentration of the substance in air	
ConWatSpg	g.m ⁻³	S	1	N	N	N	0.0 -	Concentration in incoming seepage water	if: FlwWatSpg not zero
table interpolate CntSysSedIni: column 1	m	A	no	N	N	Y	0.0 -	Depth in sediment	maximally 100 values
table interpolate CntSysSedIni: column 2	mg.kg ⁻¹	A	no	N	N	Y	0.0 -	Substance content	maximally 100 values
Section 8									
OptDelOutFiles	-	S	1	N	N	N	Yes,No	Swith for removing *.out files after run	
DateFormat	-	S	1	N	N	N	DaysFromSta, DaysFrom1900, Years	Date format	
RealFormat	-	S	1	N	N	N		Number format of the reals	
OptReport	-	S	1	N	N	N	FOCUS	Options for report type	
ExposureReport	-	S	1	N	N	N	Yes,No	Exposure report	
PercentileReport	-	S	1	N	N	N	No	Percentile report	not relevant for FOCUS
ThiLayTgt	m	S	1	N	N	N	0.00001 1	Thickness of target layer of sediment	
table HorizontalProfiles: column 1	-	A	no	N	N	N	StartTim EndTim		maximally every hour in simulation
OptOutputDistances	-	S	1	N	N	N	None, All, table	Switch output distances	
table OutputDistances: column 1	m	A	no	N	Y	N	0.0 -	Distance	maximally 1000 values

ID	Units	Limits on value					Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth		
table OutputDepths: column 1	m	A	no	N	N	Y	0.0 -	Depth maximally 1000 values
print_DepWat	m	S	1	N	N	N	Yes,No	Water depth
print_QBou	m ³ .s ⁻¹	S	1	N	N	N	Yes,No	Discharge
print_VelWatFlw	m.d ⁻¹	S	1	N	N	N	Yes,No	Flow velocity
print_VvrLiqDra	m.hr ⁻¹	S	1	N	N	N	Yes,No	Drain flow
print_VvrLiqRnf	m.hr ⁻¹	S	1	N	N	N	Yes,No	Runoff (+ infiltration) flow
print_FlmDra	g.m ⁻² .hr ⁻¹	S	1	N	N	N	Yes,No	Drain substance flux
print_FlmRnf	g.m ⁻² .hr ⁻¹	S	1	N	N	N	Yes,No	Runoff substance flux
print_FlmErs	g.m ⁻² .hr ⁻¹	S	1	N	N	N	Yes,No	Erosion substance flux
print_ConLiqWatLay	g.m ⁻³	S	1	N	N	N	Yes,No	Concentration in water, hour average
print_ConLiqWatLayCur	g.m ⁻³	S	1	N	N	N	Yes,No	Concentration in water, at end hour
print_CntSorMph	g.kg ⁻¹	S	1	N	N	N	Yes,No	Content sorbed to macrophytes
print_CntSorSusSol	g.kg ⁻¹	S	1	N	N	N	Yes,No	Content sorbed suspended solids
print_ConSysWatLay	g.m ⁻³	S	1	N	N	N	Yes,No	Total concentration in water
print_ConLiqSed	g.m ⁻³	S	1	N	N	N	Yes,No	Concentration in pore water sediment
print_CntSorSed	g.kg ⁻¹	S	1	N	N	N	Yes,No	Content sorbed to sediment
print_ConSysSed	g.m ⁻³	S	1	N	N	N	Yes,No	Total content in sediment
print_CntSedTgt	g.kg ⁻¹	S	1	N	N	N	Yes,No	Total content in target layer sediment
print_ConLiqSedTgt	g.m ⁻³	S	1	N	N	N	Yes,No	Concentration in pore water in target layer sediment
print_CntSorSedTgt	g.kg ⁻¹	S	1	N	N	N	Yes,No	Content sorbed in target layer sediment
print_VolErrWatLay	m ³	S	1	N	N	N	Yes,No	Volume error in waterbody
print_AmaWatLay	g	S	1	N	N	N	Yes,No	Mass in water layer
print_AmaLiqWatLay	g	S	1	N	N	N	Yes,No	Mass in liquid phase in water layer
print_AmaSorSusSol	g	S	1	N	N	N	Yes,No	Mass sorbed to suspended solids in water layer
print_AmaSorMph	g	S	1	N	N	N	Yes,No	Mass sorbed to macrophytes in water layer
print_AmaSed	g	S	1	N	N	N	Yes,No	Mass in sediment layer
print_AmaLiqSed	g	S	1	N	N	N	Yes,No	Mass in liquid phase in sediment layer
print_AmaSorSed	g	S	1	N	N	N	Yes,No	Mass sorbed in sediment layer
print_AmaDrfWatLay	g	S	1	N	N	N	Yes,No	Mass entered water layer by spray drift

ID	Units						Limits on value	Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth			
print_AmaAtmDepWatLay	g	S	1	N	N	N	Yes,No	Mass entered water layer by atmospheric depositon	not relevant for FOCUS
print_AmaDraWatLay	g	S	1	N	N	N	Yes,No	Mass entered water layer by drainage	
print_AmaRnoWatLay	g	S	1	N	N	N	Yes,No	Mass entered water layer by runoff	
print_AmaSedInWatLay	g	S	1	N	N	N	Yes,No	Mass penetrated into sediment from water layer	
print_AmaSedOutWatLay	g	S	1	N	N	N	Yes,No	Mass transfered from sediment into water layer	
print_AmaDwnWatLay	g	S	1	N	N	N	Yes,No	Mass flowed across downstream boundary out of water layer	
print_AmaUpsWatLay	g	S	1	N	N	N	Yes,No	Mass flowed across upstream boundary into water layer	
print_AmaTraWatLay	g	S	1	N	N	N	Yes,No	Mass transformed in water layer	
print_AmaForWatLay	g	S	1	N	N	N	Yes,No	Mass formed in water layer	
print_AmaVolWatLay	g	S	1	N	N	N	Yes,No	Mass volatilised in water layer	
print_AmaErrWatLay	g	S	1	N	N	N	Yes,No	Mass error in water layer	
print_AmaTraSed	g	S	1	N	N	N	Yes,No	Mass transformed in sediment layer	
print_AmaForSed	g	S	1	N	N	N	Yes,No	Mass formed in sediment layer	
print_AmaWatLayInSed	g	S	1	N	N	N	Yes,No	Mass transfered into water layer from sediment layer	
print_AmaWatLayOutSed	g	S	1	N	N	N	Yes,No	Mass transfered from water layer into sediment layer	
print_AmaDwnSed	g	S	1	N	N	N	Yes,No	Mass leaving sediment layer across lower boundary	
print_AmaErsSed	g	S	1	N	N	N	Yes,No	Mass entering sediment layer by erosion	
print_AmaErrSed	g	S	1	N	N	N	Yes,No	Mass error in sediment layer	
print_ConLiqWatNLAvg	g.m ⁻³	S	1	N	N	N	Yes,No	Concentration in water, average in evaluation stretch	not relevant for FOCUS
Print_DepWatRepCha	m	S	1	N	N	N	Yes,No	Water depth representative channel	

Annex 3 Technical description of the comprehensive output file.

ID	Units						Limits on value	Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth			
table HorizontalProfiles: column 1	-	A	no	N	N	N	StartTim EndTim	Time output horizontal profile	Maximally all hours in simulation
OptOutputDistances	-	S	1	N	N	N	None, All, table	Switch output distances	
table OutputDistances: column 1	m	A	400	N	Y	N	0.0 -	Distance	
table OutputDepths: column 1	m	A	400	N	N	Y	0.0 -	Depth	
DepWat	m	A	400	N	Y	N	Yes,No	Water depth	
QBou	m ³ .s ⁻¹	A	400	N	Y	N	Yes,No	Discharge	
VelWatFlw	m.d ⁻¹	A	400	N	Y	N	Yes,No	Flow velocity	
VvrLiqDra	m.hr ⁻¹	A	400	N	Y	N	Yes,No	Drain flow	
VvrLiqRnf	m.hr ⁻¹	A	400	N	Y	N	Yes,No	Runoff (+ infiltration) flow	
FImDra	g.m ⁻² .hr ⁻¹	A	400	N	Y	N	Yes,No	Drain substance flux	
FImRnf	g.m ⁻² .hr ⁻¹	A	400	N	Y	N	Yes,No	Runoff substance flux	
FImErs	g.m ⁻² .hr ⁻¹	A	400	N	Y	N	Yes,No	Erosion substance flux	
ConLiqWatLay_[name]	g.m ⁻³	A	400	Y	Y	N	Yes,No	Concentration in water, hour average	
ConLiqWatLayCur_[name]	g.m ⁻³	A	400	Y	Y	N	Yes,No	Concentration in water, at end hour	
CntSorMph_[name]	g.kg ⁻¹	A	400	Y	Y	N	Yes,No	Content sorbed to macrophytes	
CntSorSusSol_[name]	g.kg ⁻¹	A	400	Y	Y	N	Yes,No	Content sorbed suspended solids	
ConSysWatLay_[name]	g.m ⁻³	A	400	Y	Y	N	Yes,No	Total concentration in water	
ConLiqSed_[name]	g.m ⁻³	A	400	Y	Y	Y	Yes,No	Concentration in pore water sediment	
CntSorSed_[name]	g.kg ⁻¹	A	400	Y	Y	Y	Yes,No	Content sorbed to sediment	
ConSysSed_[name]	g.m ⁻³	A	400	Y	Y	Y	Yes,No	Total content in sediment	
CntSedTgt_[name]	g.kg ⁻¹	A	400	Y	N	N	Yes,No	Total content in target layer sediment	
ConLiqSedTgt_[name]	g.m ⁻³	A	400	Y	N	N	Yes,No	Concentration in pore water in target layer sediment	
CntSorSedTgt_[name]	g.kg ⁻¹	A	400	Y	N	N	Yes,No	Content sorbed in target layer sediment	
VolErrWatLay	m ³	S	1	N	N	N	Yes,No	Volume error in waterbody	
AmaWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass in water layer	
AmaLiqWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass in liquid phase in water layer	
AmaSorSusSol_[name]	g	S	1	Y	N	N	Yes,No	Mass sorbed to suspended solids in water layer	

AmaSorMph_[name]	g	S	1	Y	N	N	Yes,No	Mass sorbed to macrophytes in water layer
AmaSed_[name]	g	S	1	Y	N	N	Yes,No	Mass in sediment layer
AmaLiqSed_[name]	g	S	1	Y	N	N	Yes,No	Mass in liquid phase in sediment layer
AmaSorSed_[name]	g	S	1	Y	N	N	Yes,No	Mass sorbed in sediment layer
AmaDrfWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass entered water layer by spray drift
AmaAtmDepWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass entered water layer by atmospheric depositon
AmaDraWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass entered water layer by drainage
AmaRnoWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass entered water layer by runoff
AmaSedInWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass penetrated into sediment from water layer
AmaSedOutWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass transfered from sediment into water layer
AmaDwnWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass flowed across downstream boundary out of water layer
AmaUpsWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass flowed across upstream boundary into water water layer
AmaTraWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass transformed in water layer
AmaForWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass formed in water layer
AmaVolWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass volatilised in water layer
AmaErrWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass error in water layer
AmaTraSed_[name]	g	S	1	Y	N	N	Yes,No	Mass transformed in sediment layer
AmaForSed_[name]	g	S	1	Y	N	N	Yes,No	Mass formed in sediment layer
AmaWatLayInSed_[name]	g	S	1	Y	N	N	Yes,No	Mass transfered into water layer from sediment layer
AmaWatLayOutSed_[name]	g	S	1	Y	N	N	Yes,No	Mass transfered from water layer into sediment layer
AmaDwnSed_[name]	g	S	1	Y	N	N	Yes,No	Mass leaving sediment layer across lower boundary
AmaErsSed_[name]	g	S	1	Y	N	N	Yes,No	Mass entering sediment layer by erosion
AmaErrSed_[name]	g	S	1	Y	N	N	Yes,No	Mass error in sediment layer
ConLiqWatNLAvg_[name]	g.m ⁻³	S	400	Y	Y	N	Yes,No	Concentration in water, average in evaluation stretch
DepWatRepCha	m	S	400	N	N	N	Yes,No	Water depth representative channel

Annex 4 The sediment section of the TOXSWA input file for substances with Koc higher than 30 000 L/kg

The values that have to be changed from the standard FOCUS segmentation are indicated in bold. This segmentation consists of 11 layers, whereas the standard FOCUS segmentation consists of 6 layers.

```
*-----
*
* Section 4: Sediment section
*-----
*

FOCUS_highKoc      SedimentTypeID  ! Name of sediment type

* table SedimentProfile
* ThiHor = thickness of horizon [0.0001 - ]
* NumLay = number of layers in horizon [1,]

table SedimentProfile
ThiHor      NumLay
(m)
0.00024    8
0.00012    2
0.00024    2
0.0009     3
0.0015     2
0.004      2
0.003      1
0.01       2
0.03       3
0.02       1
0.03       1
end_table

Input            OptSedProperties  ! Option sediment properties [Input, Calc]

* table specifying SedimentProperties for each horizon:
* Nr             = number horizon [1,]
* Rho            = bulk density [100 - 2000]
* CntOm          = organic matter mass content [0.1 - 1.0]
* ThetaSat       = saturated water content [0.1 - 0.95]
* CofDifRel      = relative diffusion coefficient [0.0 - 1.0]

table horizon SedimentProperties
Nr      Rho      CntOm      ThetaSat  CofDifRel
        (kg.m-3) (kg.kg-1) (m3.m-3)  (-)
1       800.     0.09      0.6      0.6
2       800.     0.09      0.6      0.6
3       800.     0.09      0.6      0.6
4       800.     0.09      0.6      0.6
5       800.     0.09      0.6      0.6
6       800.     0.09      0.6      0.6
7       800.     0.09      0.6      0.6
8       800.     0.09      0.6      0.6
9       800.     0.09      0.6      0.6
10      800.     0.09      0.6      0.6
11      800.     0.09      0.6      0.6
end_table

0.              FlwWatSpg (m3.m-2.d-1)

* If: FlwWatSpg not zero

* table horizon DispersionLength
* Nr             = Horizon number []
* LenDisSedLiq   = Dispersion length of solute in liquid phase [0.05 - 1.0]

table horizon DispersionLength
Nr      LenDisSedLiq
        (m)
1       0.015
2       0.015
3       0.015
4       0.015
5       0.015
```

```

6          0.015
7          0.015
8          0.015
9          0.015
10         0.015
11         0.015
end_table

* If: OptLoa = PRZM
0.01          ThiLayErs (m)          ! Thickness of sediment layer to which eroded soil is added
[0.0001 - ]

```


Annex 5 The TOXSWA input file for the example water-sediment study

```

*-----
* TOXSWA input file
* INPUT FILE for TOXSWA 3 version (f90)
*-----
* This file is intended to be used by expert users.
*
* Contact address:
* -----
* Wim Beltman
* Alterra
* PO BOX 47
* 6700 AA Wageningen
* The Netherlands
* e-mail: wim.beltman@wur.nl
*
* (c) Alterra
*
*-----
*
* Section 1: Control Section
*-----
*
01-Jan-1985      TimStart      ! Start date of simulation [01-Jan-1900 - 31-Dec-9999]
01-May-1985      TimEnd        ! End date of simulation [01-Jan-1900 - 31-Dec-9999]
FOCUS            CallingProgram ! Calling program in FOCUS_TOXSWA for EU authorization
4                CallingProgramVersion ! Version of calling program
4                ModelVersion    ! version number of the model
4                GUIVersion      ! version number of the GUI
2                DBVersion       ! version number of the database
Hourly           OptInp         ! Option for hourly or daily input data (Hourly, Daily)
OnLine           OptHyd         ! Hydrology simulation option (Only,OnLine,OffLine,Automatic)
OnLine           OptTem         ! Temperature simulation option (Only,OnLine,OffLine Automatic)
600              MaxTimStpWat (s) ! Maximum calculation time step in water layer [0.001 - 3600]
600              MaxTimStpSed (s) ! Maximum calculation time step in sediment [0.001 - 3600]
600.             TimStpHyd (s)   ! Maximum calculation time step for hydrology [0.001 - 3600]
No               OptScreen      ! Option to show output on screen (Yes, No)
Calc             OptTimStp      ! Time step substance simulation options (Input, Calc)

*-----
*
* Section 2: Waterbody section
*-----
*
C3river_WS       Location      ! Name of the location
C3river_WS       WaterbodyID   ! ID of the water body

* Table WaterBody
* Len            = Length (m) [0.1 - 10000]
* NumSeg         = Number of segments (-) [1 - 1000]
* WidWatSys      = Width of the bottom of water system (m) [0.1 - 100]
* SloSidWatSys   = Side slope of the water system (-) [0.001 - 2]
* DepWatDefPer   = Water depth defining perimeter for the exchange between water layer and sediment (m) [0
- lowest water depth]

table WaterBody
Len      NumSeg  WidWatSys SloSidWatSys DepWatDefPer
(m)      (-)    (m)        (-)         (m)
1.        1      1.         0.          0.
End_table

0.         ConSus (g.m-3)      ! Concentration of suspended solids [1.0 - 100000]
0.         CntOmSusSol (kg.kg-1) ! Mass ratio of organic matter in suspended solids [0.0
0.         AmaMphWatLay (g.m-2) ! Dry weight of macrophyte biomass per m2 bottom [0.0 -

*-----
*
* Section 3: Hydrology: general
*-----
*
Constant    OptWaterSystemType ! Option for selecting the water system type (Pond, WaterCourse)
Constant    OptFloWat          ! Option for water flow (Constant, Variable)

* if: OptWaterSystemType = WaterCourse
Fischer     OptDis             ! Options are 'Fischer' and 'Input'

* if: OptDis = Input
9.88131291682493E-324 CofDisPhsInp (m2.d-1) ! Dispersion coefficient [0. - 100000]
*-----

```

```

*
* Section 3a: Constant water flow
*-----
*
* if: OptFloWat = Constant
0.06          DepWat (m)
0.           VelWatFlwBas (m.d-1)
*-----
*
* Section 3b: Variable water flow: pond
*-----
*
* if: OptFloWat = Variable and OptWaterSystemType = Pond
0.45          AreaSurPndInp (ha)      ! Size of area surrounding the pond [0.0 - 50.0]
*-----
*
* if: CallingProgram = FOCUS
2.193         QBasPndInp (m3.d-1)      ! Base flow, i.e. inflow into pond [0.001 - 50.0]
1.           HgtCrePnd (m)             ! Height of the weir crest [0.1 - 5.0]
0.5          WidCrePnd (m)             ! Width of the weir crest [0.01 - 10]
*-----
*
* if: Opt = Runoff
0.06          AreaErsSurPndInp (ha)    ! Size of the eroding area around the pond [0.0 - 50.0]
*-----
*
* Section 3c: Variable water flow: watercourse
*-----
*
* if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
*representative channel
0.0001        SloBotRepCha (-)          ! Slope bottom representative channel [0.0 - 0.01]
0.4           HgtCreRepCha (m)          ! Height of the weir crest [0.1 - 5.0]
0.5           WidCreRepCha (m)          ! Width of the weir crest [0.01 - 10]
*-----
1000.         LenRepCha (m)             ! Length representative channel [10.0 - 2000]
1.           WidBotRepCha (m)          ! Width bottom representative channel [0.1 - 10]
1E-005        SloSidRepCha (-)          ! Side slope of the representative channel [0.0 - 10]
*-----
25.           CofRghRef (-)            ! Value of the Manning coefficient for bottom roughness [1.0-100]
1.2          CofVelHea (-)            ! Energy coefficient resulting from the non-uniform distribution
*-----
*
* if: CallingProgram = NL or FOCUS
2.           AreaUpsWatCrsInp (ha)      ! Size of the area upstream the representative channel
0.66         QBasWatCrsInp (m3.d-1)     ! Minimal flow into watercourse [0.0 10000]
2.           AreaUpStrRepCha (ha)       ! Size of the area upstream the representative channel
1.           QBasRepCha (m3.d-1)        ! Minimal flow into watercourse [0.0 - 10000]
*-----
*
* Section 4: Sediment section
*-----
*
C3river_WS-sediment  SedimentTypeID    ! Name of sediment type
*
* table SedimentProfile
* ThiHor = thickness of horizon [0.0001 - ]
* NumLay = number of layers in horizon [1,]
*
table SedimentProfile
ThiHor      NumLay
(m)
0.00024     8
0.00012     2
0.00024     2
0.0009      3
0.0015      2
0.004       2
0.003       1
0.015       3
end_table
*
Input          OptSedProperties          ! Option sediment properties [Input, Calc]
*
* table specifying SedimentProperties for each horizon:
* Nr          = number horizon [1,]
* Rho         = bulk density [100 - 2000]
* CntOm       = organic matter mass content [0.1 - 1.0]
* ThetaSat    = saturated water content [0.1 - 0.95]
* CofDifRel   = relative diffusion coefficient [0.0 - 1.0]
*
table horizon SedimentProperties
Nr          Rho          CntOm      ThetaSat  CofDifRel
            (kg.m-3)     (kg.kg-1) (m3.m-3)  (-)
1           1536.        0.016    0.417     0.364
2           1536.        0.016    0.417     0.364
3           1536.        0.016    0.417     0.364
4           1536.        0.016    0.417     0.364
5           1536.        0.016    0.417     0.364
6           1536.        0.016    0.417     0.364
7           1536.        0.016    0.417     0.364
8           1536.        0.016    0.417     0.364
end_table

```

```

0.                FlwWatSpG (m3.m-2.d-1)

* If: FlwWatSpG not zero
* table horizon DispersionLength
* Nr                = Horizon number []
* LenDisSedLiq     = Dispersion length of solute in liquid phase [0.05 - 1.0]

table horizon DispersionLength
Nr                LenDisSedLiq
                (m)
1                 0.05
2                 0.05
3                 0.05
4                 0.05
5                 0.05
6                 0.05
7                 0.05
8                 0.05
end_table

* If: OptLoa = PRZM
0.01              ThiLayErs (m)          ! Thickness of sediment layer to which eroded soil is added
[0.0001 - ]
*-----
*
* Section 5: Weather section
*-----
*

WS                MeteoStation          ! Name of the *.met file with meteo data

Monthly           OptMetInp             ! Option for hourly or daily input data (Hourly, Daily, Monthly)

*-----
*
* Section 6: Compound section
*-----
*

WTSD1             SubstanceName          ! Name of parent substance [1 - 6 characters]

table compounds                                       ! List of substances [1 - 6 characters]
WTSD1
end_table

* Table parent-daughter relationships transformation in water (FraPrtDauWat):
* Column 1: fraction formed from parent into daughter
* Column 2: name of parent
* Column 3: name of daughter

table FraPrtDauWat (mol.mol-1)
end_table

* Table parent-daughter relationships transformation in sediment (FraPrtDauSed):
* Column 1: fraction formed from parent into daughter
* Column 2: name of parent
* Column 3: name of daughter

Table FraPrtDauSed (mol.mol-1)
end_table

* Substance properties for each substance given in table compounds
* Substance code is extension of parameter name
*----- Parent: WTSD1 -----

418.9             MolMas_WTSD1 (g.mol-1) ! Molar mass of parent substance [10.0 - 10000]

0.84              DT50WatRef_WTSD1 (d)   ! Half-life transformation in water [0.1 - 100000]
20.               TemRefTraWat_WTSD1 (C) ! Temperature at which half-life was measured [5.0 - 30]
55.               MolEntTraWat_WTSD1 (kJ.mol-1) ! Molar activation enthalpy of transformation in
590.              DT50SedRef_WTSD1 (d)   ! Half-life transformation in sediment [0.1 - 100000]
20.               TemRefTraSed_WTSD1 (C) ! Temperature at which half-life was measured [5.0 - 30]
55.               MolEntTraSed_WTSD1 (kJ.mol-1) ! Molar activation enthalpy of transformation in

44083.5266821346 KomSed_WTSD1 (L.kg-1) ! Coefficient of equilibrium sorption in sediment [0.0 -
1.                ConLiqRefSed_WTSD1 (mg.L-1) ! Reference concentration in liquid phase in
0.9               ExpFreSed_WTSD1 (-)    ! Freundlich exponent in sediment [0.1 - 2]
44083.5266821346 KomSusSol_WTSD1 (L.kg-1) ! Coefficient of equilibrium sorption suspended
1.                ConLiqRefSusSol_WTSD1 (mg.L-1) ! Reference concentration in liquid phase
0.9               ExpFreSusSol_WTSD1 (-) ! Freundlich exponent suspended solids [0.1 - 2]
0.                CofSorMph_WTSD1 (L.kg-1) ! Coefficient for linear sorption on macrophytes [0.0

1.7E-7            PreVapRef_WTSD1 (Pa) ! Saturated vapour pressure [0.0 - 200000]
20.               TemRefVap_WTSD1 (C) ! Temperature of reference at which the saturated vapour
95.               MolEntVap_WTSD1 (kJ.mol-1) ! Molar enthalpy of the vaporization process [-200 -
200]

7.5               SlbWatRef_WTSD1 (mg.L-1) ! Water solubility [0.001 - 1000000]
25.               TemRefSlb_WTSD1 (C) ! Temperature of reference at which the water solubility
27.               MolEntSlb_WTSD1 (kJ.mol-1) ! Molar enthalpy of the dissolution [-200 - 200]
4.3E-5            CofDifWatRef_WTSD1 (m2.d-1) ! Reference diffusion coefficient in water [0.0 -

```

```

*-----
*
* Section 7: Management section
*-----
*

* Loading options (OptLoa):
* DriftOnly = spray drift only entry route
* PEARL     = drainage calculated by PEARL
* MACRO     = drainage calculated by MACRO
* PRZM      = runoff and erosion calculated by PRZM
* GEM       = point source calculated by GEM

DriftOnly          OptLoa          ! Loading options (DriftOnly, PEARL, MACRO, PRZM, GEM)

FOCUS_EXAMPLE ApplicationScheme ! Name of the application scheme

* Table loadings
* Column 1: Date of application, relevant if OptLoa = DriftOnly, otherwise the date is a dummy values
* Column 2: Type of loading (-)
* Column 3: Drift deposition (mg.m-2) []
* Column 4: Start of stretch of watercourse loaded by all loading types (m) []
* Column 5: End of stretch of watercourse loaded by all loading types (m) []

table Loadings
end_table

* If: OptLoa = MACRO or OptLoa = PRZM
* Table with path+name of lateral entries files

table Soil substance files
end_table

* If: OptLoa = PEARL or OptLoa = MACRO
100.          WidFldDra (m)          ! Width of field contributing drainage

* If: OptLoa = PRZM
100.          WidFldRnf (m)          ! Width of field contributing runoff
20.           WidFldErs (m)          ! Width of field contributing erosion
0.            RatInfDir (-)          ! Ratio of infiltration water added to runoff water

* If: CallingProgram = FOCUS and OptWaterSystemType = WaterCourse
Yes           OptUpsInp              ! Switch for upstream catchment treated (Yes, No)

0.            RatAreaUpsApp (-)       ! Ratio of upstream catchment treated [0.0 - 1]
1.            FraMetForUps (-)        ! Fraction primary metabolites formed in water in upstream
catchment
0.            ConAir (kg.m-3)          ! Concentration of the substance in air
0.            ConWatSpg (g.m-3)       ! Concentration in incoming seepage water

0.013881      ConSysWatIni (g.m-3)

* Table initial substance content in sediment (CntSysSedIni)
* Column 1: Depth in sediment (m)
* Column 2: Substance content (mg.kg-1)
table interpolate CntSysSedIni (mg.kg-1)
end_table

*-----
*
* Section 8: Output control
*-----
*

No             OptDelOutFiles          ! Switch for removing *.out files after run (Yes, No)
FOCUS          OptReport               ! Options for report type (DutchRegistration, FOCUS)
Yes            ExposureReport          ! Exposure report (Yes, No)
No             PercentileReport        ! Percentile report (Yes, No)
DaysFromSta    DateFormat              ! Date format (DaysFromSta, DaysFrom1900, Years)
e14.6          RealFormat              ! Number format of the reals

0.025          ThiLayTgt (m)           ! Thickness of the target layer
Hour           OptDelTimPrn            ! Option to set output time step (Hour, Day, Decade, Month, Year,
1              DelTimPrn (d)           ! Output time step [0.0 - length simulation period]
No             PrintCumulatives        ! Specify whether fluxes should be cumulated over the entire
simulation period (Yes, No)

* table HorizontalProfiles: dates are given for which detailed output is wished
* Column 1: dates
table HorizontalProfiles
end_table

* Table output depths (OutputDepths): indicate for which depths the output is selected
* Column 1: Depth
table OutputDepths (m)
end_table

All OptOutputDistances ! Switch output distances (None, All, Table)

* Table output distances (OutputDistances): indicate for which distance the output is selected
* Column 1: Distance
table OutputDistances (m)
end_table

```

No	print_VelWatFlw	! Flow velocity (m/h) [Yes, No]
No	print_QBou	! Discharge (m3/h) [Yes, No]
No	print_VvrLiqDra	! Drain flow (m/h) [Yes, No]
No	print_VvrLiqRnf	! Runoff flow [Yes, No]
No	print_FlmDra	! Drain substance flux [Yes, No]
No	print_FlmRnf	! Runoff substance flux [Yes, No]
No	print_FlmErs	! Erosion substance flux [Yes, No]
Yes	print_ConLiqWatLay	! Concentration in water, hour average (g/m3) [Yes,
No	print_ConSysWatLay	! Total concentration in water (g/m3) [Yes, No]
No	print_CntSorMph	! Content sorbed to macrophytes [Yes, No]
No	print_CntSorSusSol	! Content sorbed suspended solids [Yes, No]
No	print_ConSysSed	! Total content in sediment [Yes, No]
No	print_ConLiqSed	! Concentration in pore water sediment (g/m3) [Yes,
No	print_CntSorSed	! Content sorbed to sediment [Yes, No]
No	print_DepWat	! Water depth (m) [Yes, No]
No	print_DepWatRepCha	! Water depth representative channel [Yes, No]
Yes	print_CntSedTgt	! Total content in target layer sediment [Yes, No]
No	print_ConLiqSedTgt	! Concentration in pore water in target layer sediment
No	print_CntSorSedTgt	! Content sorbed in target layer sediment [Yes, No]
Yes	print_ConLiqWatLayCur	! Concentration in water, at end hour (g/m3)[Yes, No]
Yes	print_AmaWatLay	! Mass in water layer [Yes, No]
Yes	print_AmaLiqWatLay	! Mass in liquid phase in water layer [Yes, No]
Yes	print_AmaSorSusSol	! Mass sorbed to suspended solids in water layer [Yes, No]
Yes	print_AmaSorMph	! Mass sorbed to macrophytes in water layer [Yes, No]
Yes	print_AmaSed	! Mass in sediment layer [Yes, No]
Yes	print_AmaLiqSed	! Mass in liquid phase in sediment layer [Yes, No]
Yes	print_AmaSorSed	! Mass sorbed in sediment layer [Yes, No]
Yes	print_AmaTraWatLay	! Mass transformed in water layer [Yes, No]
Yes	print_AmaForWatLay	! Mass formed in water layer [Yes, No]
Yes	print_AmaVolWatLay	! Mass volatilised in water layer [Yes, No]
Yes	print_AmaSedInWatLay	! Mass penetrated into sediment from water layer [Yes, No]
Yes	print_AmaSedOutWatLay	! Mass transferred from sediment into water layer [Yes, No]
Yes	print_AmaDwnWatLay	! Mass flowed across downstream boundary out of water
Yes	print_AmaUpsWatLay	! Mass flowed across upstream boundary into water
Yes	print_AmaDrfWatLay	! Mass entered water layer by spray drift [Yes, No]
Yes	print_AmaAtmDepWatLay	! Mass entered water layer by atmospheric deposition
Yes	print_AmaDraWatLay	! Mass entered water layer by drainage [Yes, No]
Yes	print_AmaRnoWatLay	! Mass entered water layer by runoff [Yes, No]
Yes	print_AmaTraSed	! Mass transformed in sediment layer [Yes, No]
Yes	print_AmaForSed	! Mass formed in sediment layer [Yes, No]
Yes	print_AmaWatLayInSed	! Mass transferred into water layer from sediment
Yes	print_AmaWatLayOutSed	! Mass transferred from water layer into sediment layer
Yes	print_AmaDwnSed	! Mass leaving sediment layer across lower boundary
Yes	print_AmaErsSed	! Mass entering sediment layer by erosion [Yes, No]
No	print_VolErrWatLay	! Volume error in waterbody [Yes, No]
No	print_AmaErrWatLay	! Mass error in mass balance of the waterlayer [Yes,
No	print_ConLiqWatLayNLAvg	! Concentration in water, average in evaluation

*-----
 * End of TOXSWA input file
 *-----

Annex 6 Sediment properties of bulk density, porosity and organic matter content, and derivation of relative diffusion coefficient

In the TOXSWA model the properties of bulk density, porosity and organic matter content need to be defined as a function of depth in the sediment. These properties may be obtained in two ways:

- (i) directly by measurements (e.g. Adriaanse *et al.*, 2014) or
- (ii) by derivation from measurements, e.g. the sediment in the FOCUS surface water scenarios, with its bulk density of 800 kg.m⁻³, porosity of 0.6 and organic matter content of 0.09 (for the entire depth of 10 cm).

From a logical point of view the values of sediment properties should fulfil Eq. A1 below, which states that the volume fractions of water, organic matter and mineral parts sum up to 1:

$$\varepsilon + \frac{\rho_{sed}}{\rho_{om}} f_{om, sed} + \frac{(1 - f_{om, sed}) \rho_{sed}}{\rho_{min}} = 1 \quad (A1)$$

where ε (L³ L⁻³) is the porosity, i.e. volume of liquid divided by volume of sediment, ρ_{sed} (M L⁻³) is the bulk density of dry sediment, i.e. mass of dry sediment per volume of sediment, ρ_{om} (M L⁻³) is the phase density of organic matter, $f_{om, sed}$ (M M⁻¹) is the mass fraction of sediment organic matter and ρ_{min} (M L⁻³) is the phase density of mineral matter.

However, when we calculated the organic matter content for a data set with 19 measurements of bulk density ρ_{sed} and porosity ε for the upper 5 cm of ditch sediment for which we had no measurements of the organic matter content, with the aid of Eq. A1 and using the values of 1.40 kg L⁻¹ for ρ_{om} and 2.65 kg L⁻¹ for ρ_{min} we obtained 9 negative $f_{om, sed}$ values out of the 19 $f_{om, sed}$ values. The average $f_{om, sed}$ value was 0.005 g g⁻¹ and the standard deviation 0.098 g g⁻¹ ($n=19$). The large standard deviation suggests that the $f_{om, sed}$ value is very sensitive to small changes in the ρ_{sed} and ε values (Adriaanse *et al.*, 2013). So, some variability in the measurements easily results in unreliable outcomes of Eq. A1. Therefore, if there is trust in the measured sediment properties, but they do not fulfil exactly Eq. A1, this does not necessarily invalidate the measurements in our view.

If the TOXSWA user has derived sediment properties instead of directly measuring them, we advise to select the properties in such a way that they do fulfil Eq. A1.

In addition, the relative diffusion coefficient (= tortuosity) can be determined as a function of the porosity, as described below.

The tortuosity factor⁶, λ , is strongly related to porosity. Boudreau (1996) derived the empirical equation $\lambda = 1/[1 - \ln(\varepsilon^2)]$ from experimental data and theoretical work. The tortuosity factor can also be estimated with the relation derived theoretically for a medium containing a mixture of different sized spherical particles as recommended for saturated soils by Nye and Tinker (1977): $\lambda = \varepsilon^{1/2}$. Also used in the past for estimation of the tortuosity factor is a table recommended by Leistra for soils (1978). These two methods, Boudreau's method and tortuosity factors calculated from measurements by Sweert *et al.* (1991) are presented in Figure A5.1. The data of Sweerts *et al.* (1991), originating from investigations of freshwater sediments, cover approximately 1/3 of the whole data set Boudreau used to fit his empirical equation. The other 2/3 of Boudreau's data set were from marine sediments.

⁶ Other authors define the product $\varepsilon\lambda$ as being the tortuosity factor or as 'the tortuosity', which causes confusion. We define tortuosity as the effect of traversing a tortuous pathway.

The study of Sweerts *et al.*, (1991) is based on experimental data of sediments from medium-sized and small lakes covering a large porosity range (0.41–0.96) and different sediment types including sand, silt, peat and flocks consisting of 0.1–37.3% organic carbon. Sweerts *et al.* (1991) suggested that the tortuosity decreased in high porosity sediments because the viscosity of the pore water was enhanced by dissolved or gel-like organic compounds, obstructing diffusion.

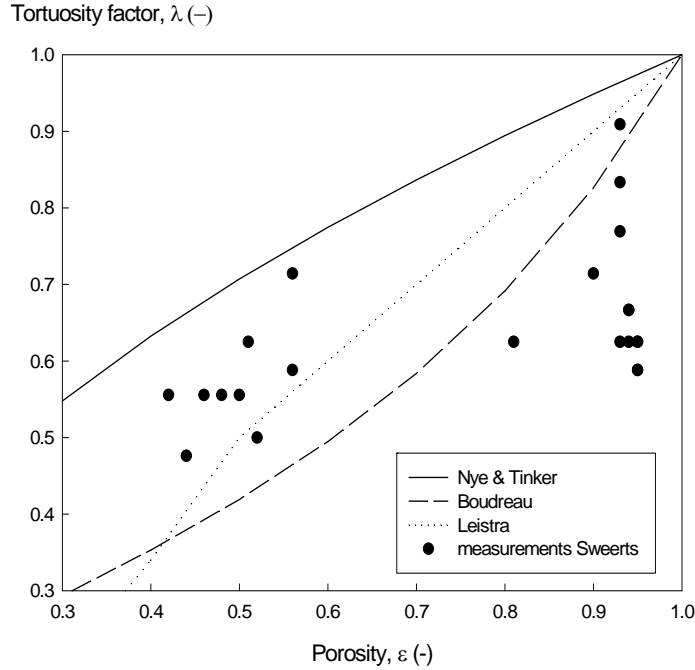


Figure A7.1 The tortuosity factor as function of porosity. The lines indicate tortuosity factors calculated with equations of Nye and Tinker (1977), of Boudreau (1996) and of Leistra (1978). The dots indicate tortuosity factors calculated by Sweerts *et al.* (1991) from measurements in freshwater sediments.

Figure A7.1 shows that at high porosities the tortuosity factors calculated with Boudreau's equation are closest to Sweet's tortuosity factors. Leistra's method describes the tortuosity factors in the middle range better than Boudreau and also better than Nye and Tinker. Nye and Tinker's equation overestimates the tortuosity factor over the whole range. Boudreau's equation is recommended for estimation of the tortuosity factor for sediments because it fits better to the tortuosity factors at high porosities and because it is based on measurements for sediments (instead of soils).

Definition of sediment properties

Eq. A1 is based upon the following definitions of phase density, bulk density, porosity and organic matter content (Koorevaar *et al.* (1983) for soil, see also Adriaanse *et al.*, 2014). Sediment is composed of organic matter, mineral matter and water; the water resides in the pores of the sediment.

Before being able to define the bulk density of the sediment we define the general notion of density or volumic mass:

$$\rho = \frac{\text{mass_of_matter}}{\text{volume_of_matter}} \quad (\text{A2})$$

with ρ = density, or volumic mass (kg m^{-3}).

So, phase density, ρ_x , (kg m^{-3}), is the mass of phase x , divided by the volume of phase x . The phase density of organic matter is $1200\text{--}1500 \text{ kg m}^{-3}$ (average = 1400 kg m^{-3}). The phase density of mineral matter is $2600\text{--}2850 \text{ kg m}^{-3}$ (average is 2700 kg m^{-3}).

Bulk density is mass of sediment divided by the total or bulk volume of the sediment, ${}^b\rho_d$, (kg m⁻³), where b stands for bulk and d for dry. So:

$${}^b\rho_d = \frac{\text{mass_solid}}{\text{bulk_volume}} = \frac{\text{mass_om} + \text{mass_min}}{\text{bulk_volume}} \quad (\text{A3})$$

with ${}^b\rho_d$, is the dry bulk density, (kg m⁻³), and the solid mass (kg) is composed of organic matter (om in kg) and minerals (min in kg). The dry bulk density is the bulk density of the sample after drying in an oven at 105°C to a constant mass, based on the original volume. The wet bulk density, ${}^b\rho_w$, (kg m⁻³), is defined by

$${}^b\rho_w = \frac{\text{mass_solid} + \text{mass_liquid}}{\text{bulk_volume}} = \frac{\text{mass_om} + \text{mass_min} + \text{mass_liquid}}{\text{bulk_volume}} \quad (\text{A4})$$

with ${}^b\rho_w$, = wet bulk density (kg m⁻³), the bulk density of the original wet sample.

The organic matter content of sediment is defined as

$$m_{om} = \frac{\text{mass_om}}{\text{mass_om} + \text{mass_min}} \quad (\text{A5})$$

with m_{om} = mass ratio of organic matter to solid phase (-). The organic matter content, m_{om} , is determined from the loss of weight of an oven-dry sample upon complete oxidation of the organic matter at about 900 °C. The solid phase is sieved before entering the oven.

The porosity of the sediment or the volume fraction of pores is defined as

$$\varphi = \frac{\text{total_volume_of_pores}}{\text{volume_of_sediment}} \quad (\text{A6})$$

with φ = porosity, volume fraction of pores in the sediment (-).

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Annex 7 Sdwin tool for transfer of selected TOXSWA output to a text file

Using this tool, records with the same identifier can be selected and exported to a text file. This text file can then be imported in a graphical program or in an Excel file. The sdwin tool (sdwin32.exe) can be obtained by sending an E-mail to toxswa-swash@wur.nl. If FOCUS_PEARL is on your computer, sdwin32.exe can also be found in the bin directory of the Pearl software. A brief description of the tool is given in this annex.

Sdwin32 uses a small configuration file (or set file). this file contains lines with selection criteria as follows:

```
<datafile_name><Column_X><Column_Y><Column_with_LookUpString><LookUpString>
```

A maximum number of 9 data pairs can be used.

For clarification the following example is given for the contents of the set file (see the format of the output file of TOXSWA):

```
3.out 1 4 3 ConLiqWatLay_Par
```

This means that the data file is 3.out, that X data are taken from column 1 and that Y data are taken from column 4. Only lines with QBou in the third column will be selected (note that the selection is case sensitive).

If the X data are in the same column for all data series, you can replace the value of Column_X with ! (except for the first data series):

```
3.out 1 4 3 ConLiqWatLay_Par
3.out ! 23 3 ConLiqWatLay_Par
3.out ! 23 3 ConLiqWatLay_Par
```

gives the following results (only first part of file shown)

```
0.021 0.393152E-03 0.802153E-04 0.528904E-05
0.063 0.984952E-03 0.676716E-03 0.286616E-03
0.104 0.101634E-02 0.975418E-03 0.823502E-03
0.146 0.101722E-02 0.100584E-02 0.979666E-03
```

Sdwin32 must be called from the command line:

```
sdwin32 setfile -o outputfile
```

where *setfile* indicates the name of the set file, and *outputfile* indicates the name of the file where the result of the selection are directed.

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ISSN 2352-2739

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