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# Manual for FOCUS\_TOXSWA v5.5.3 and for expert use of TOXSWA kernel v3.3

User's Guide version 5

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

| WOt-technical report 126



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**Manual for FOCUS\_TOXSWA v5.5.3 and for expert use of TOXSWA kernel v3.3**

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**Statutory Research Tasks Unit for Nature & the Environment**

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## Abstract

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The FOCUS\_TOXSWA model calculates exposure concentrations of pesticides and their metabolites in watercourses and ponds, of the so-called FOCUS surface water scenarios. These concentrations are used in the pesticide registration procedure at EU level. The model concepts of TOXSWA are described briefly. The procedure for using the TOXSWA kernel (i.e. expert use) and related input files and output files are described. Concerning FOCUS\_TOXSWA, the use of the graphical user interface to access the input and output is 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: pesticides, metabolites, exposure concentration, TOXSWA, FOCUS, surface water, sediment*

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# Preface

This manual replaces the manual which was provided with FOCUS\_TOXSWA 4.4.2 and FOCUS\_TOXSWA 4.4.3. Some improvements were made in the version of FOCUS-TOXSWA 5.5.3 (released in 2018). Therefore the manual was updated to comply with this FOCUS\_TOXSWA version. The result is the current manual for use of FOCUS\_TOXSWA 5.5.3. In this update a more explicit distinction is made between expert use of the TOXSWA kernel and use of the FOCUS\_TOXSWA software for use with the FOCUS surface water scenarios. The authors hope the manual will be of use; assisting first-time users in their first endeavours, and serving as a reference for more advanced users.

*Wim Beltman, Mechteld ter Horst, Paulien Adriaanse en Arjan de Jong*



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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 5.5.3 model. The most important new features of the FOCUS\_TOXSWA model compared to the previous FOCUS\_TOXSWA versions 4.4.2 and 4.4.3 are:

- The format of the TOXSWA input file (runID.twx) has been restructured.
- The TOXSWA shell provides an option for running the TOXSWA model simultaneously on multiple cores of a computer with a multicore processor.

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 the TOXSWA kernel has been included as well. The input and output files are described in detail.

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



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# 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):

- De template van het TOXSWA-invoerbestand (runID.twx) is verbeterd.
- De TOXSWA Graphical User Interface heeft een optie voor het tegelijkertijd draaien van het TOXSWA-model op meerdere processoren van een computer met een multikernprocessor.

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.

Dit rapport bevat een handleiding voor de opdrachtregel-gestuurde versie van het TOXSWA-rekenhart. De invoer- en uitvoerbestanden zijn in detail beschreven.

In een afzonderlijk hoofdstuk wordt toegelicht hoe de simulaties voor een water – sedimentstudie en voor een meerjarige simulatie worden opgezet.



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# 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. Also for expert users a guide is given for use of the TOXSWA kernel.

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 (Van den Berg *et al.*, 2015). 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 5.5.3, consisting of:

TOXSWA model	FOCUS version 5 (= 3.3.6.F5, December 2017)
TOXSWA shell	FOCUS version 5 (= 4.0.0 December 2017)
SWASH/TOXSWA database	FOCUS version 3 (= April 2015)

FOCUS\_TOXSWA version 5.5.3 is linked to the FOCUS-SWASH version 5.3, consisting of:

SWASH model = shell	FOCUS version 5 (= 5.1.0, April 2015)
SWASH/TOXSWA database	FOCUS version 3 (= April 2015)

FOCUS\_TOXSWA version 5.5.3 and FOCUS-SWASH version 5.3 are linked to SPIN 2.2 consisting of:

SPIN model = shell	SPIN version 2 (= 1.2.0, December 2014)
SPIN database	SPIN version 2 (= 62, December 2014)

FOCUS\_TOXSWA v.5.5.3 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.

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## 1.2 Main improvements in FOCUS\_TOXSWA 5.5.3

The main improvements in FOCUS\_TOXSWA 5.5.3 are:

- The format of the TOXSWA input file (runID.twx) has been restructured.
- For runs with a problem due to the numerical discretization of the water layer or the sediment solutions have been designed, and were implemented in this version.
- The TOXSWA shell provides an option for running the TOXSWA model simultaneously on multiple cores of a computer with a multicore processor.
- A time-weighted average concentration over 3 d, the TWAEC\_3\_days has been added to the output file Runid.sum, in accordance with the recommendations of the Aquatic Guidance document by EFSA (2013).

With version 4.4.2 (the predecessor of version 5.5.3) some major improvements were made, compared to older versions of TOXSWA. For completeness, these improvement are described here as well.

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.

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.

FOCUS\_TOXSWA 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.

Also available is TOXSWA version 1.2, which is used in the Dutch 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 <https://esdac.jrc.ec.europa.eu/projects/toxswa>, the website of the Joint Research Centre of the EU. Note 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.

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If you encounter problems in the installation of TOXSWA, contact us at [toxswa-swash@wur.nl](mailto: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 <https://esdac.jrc.ec.europa.eu/projects/focus-dg-sante>.

## 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](mailto:toxswa-swash@wur.nl).

For errors related to running FOCUS scenarios, please contact:

[focus.helpdesk@jrc.it](mailto:focus.helpdesk@jrc.it)

## 1.5 Documentation

This manual gives guidance for the use of FOCUS\_TOXSWA 5.5.3, 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 Ter Horst *et al.* (2016) and Adriaanse (1996, 1997). A sensitivity analysis of the first version of TOXSWA (1.0), released in 1996, is reported by Westein *et al.* (1998). The theory of hydrology applied in FOCUS surface water scenarios is also given Adriaanse *et al.* (2017). The theory and numerical solutions of the hydrology used for the FOCUS surface water scenarios are described in more detail 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). TOXSWA can be used to fit the degradation rates for transformation in water from microcosms (Deneer *et al.*, 2015).

FOCUS\_TOXSWA will often be used in combination with SWASH and SPIN. The use of SWASH is reported by Van den Berg *et al.* (2015). A programmer's guide of SWASH is made by Te Roller *et al.* (2015). The use of SPIN is reported by Van Kraalingen *et al.* (2013).

## 1.6 Performed tests

TOXSWA kernel 3.3 results were compared with results of analytical solutions derived in Section 7.3 of Adriaanse (1996). The concentrations calculated in water for a constant flow simulation and the calculated contents in sediment from diffusive transport agreed well with the results of the analytical solutions. The Predicted Exposure Concentrations (PECs) calculated for a set of example runs (all FOCUS scenarios with two substances) were compared with the PECs calculated with the previous

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version released, FOCUS\_TOXSWA 4.4.3. The test results can be found in the download package of FOCUS\_TOXSWA 5.5.3 (at <https://esdac.jrc.ec.europa.eu/projects/toxswa>). The TOXSWA kernel 3.3 was also tested using a test protocol for checking the different applications of TOXSWA in software packages, and critical runs with minimum and maximum values of the most important substance parameters. Results of the runs (TOXSWA kernel 3.3.6 of FOCUS\_TOXSWA 5.5.3) were the same as results of the former version (TOXSWA kernel 3.3.4 of FOCUS\_TOXSWA 4.4.3).

The performance of the user interface of FOCUS\_TOXSWA 5.5.3 was verified using a test protocol for verification of the functionalities of the FOCUS\_TOXSWA user interface.

Test results can be requested via sending a mail to [toxswa-swash@wur.nl](mailto:toxswa-swash@wur.nl).

## 1.7 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 the TOXSWA kernel. The ASCII input files and the output files, made by TOXSWA during a simulation, are discussed. Chapter 4 is the user's 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. Note that the procedure described for setting up a calculation for a water-sediment study is similar to setting up the simulation of a cosm study, e.g. for fitting the degradation rate (see Deneer *et al.*, 2015).

## 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.

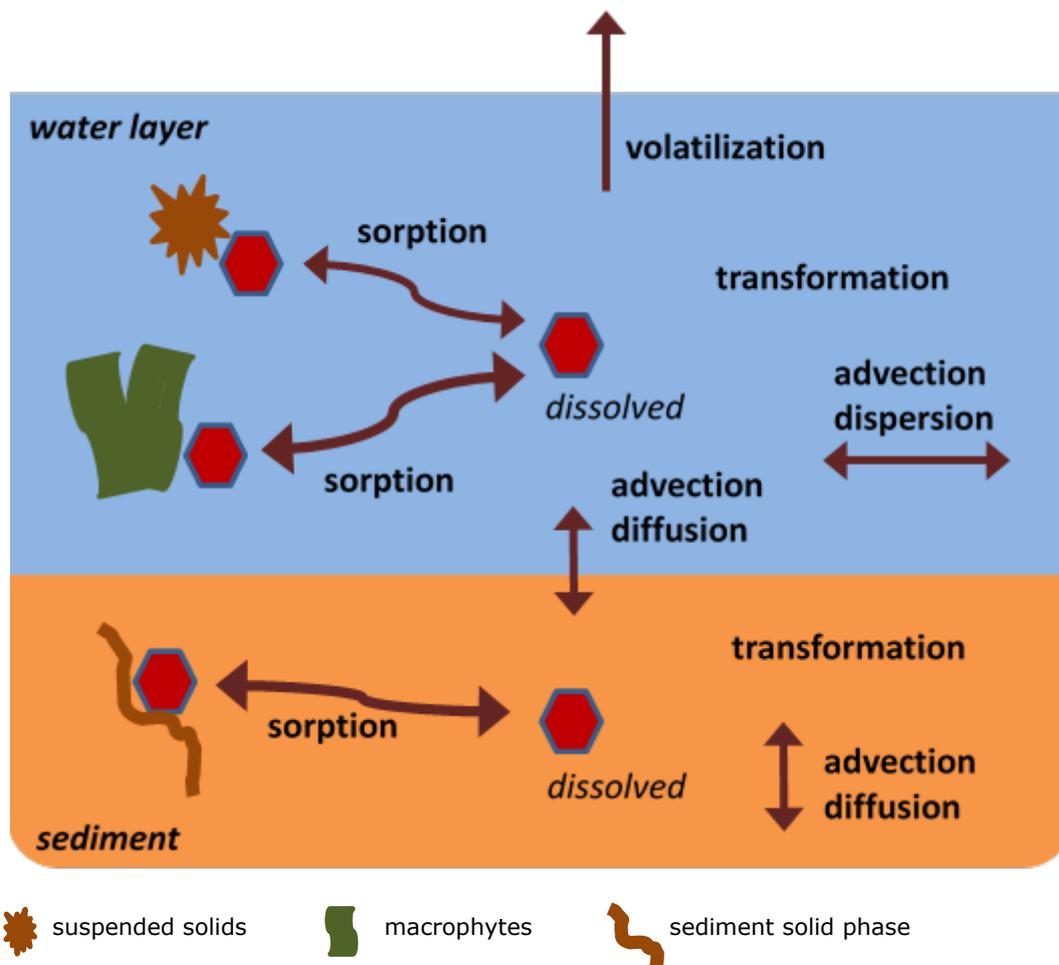


Figure 2.1 Processes in TOXSWA

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 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 (see Figure 2.2). Distances between the nodes in the water and sediments are in the order of magnitude of metres and millimetres, respectively.

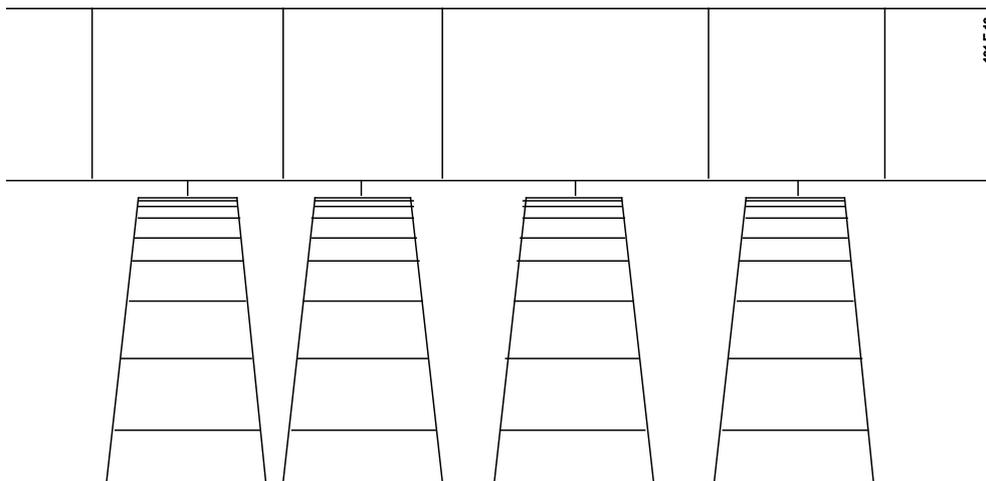


Figure 2.2 Structure of the TOXSWA water body system: one water layer subsystem and many sediment subsystems

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 by Adriaanse *et al.* (2017), Ter Horst *et al.*, (2016), and more in detail by 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.

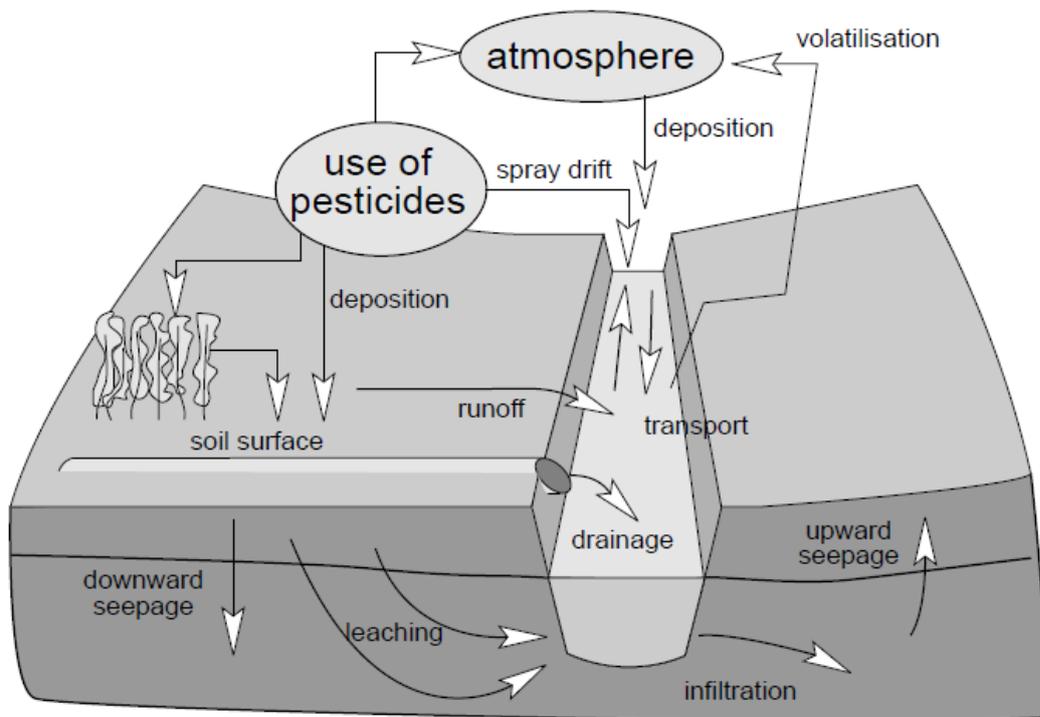


Figure 2.3 Possible entry routes of pesticides into field ditches

## 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 TOXSWA

This chapter describes the command-line version of TOXSWA. The command-line version is of interest for those who want to use FOCUS\_TOXSWA without using the User Interface, or to use TOXSWA with other applications. The command-line version is also 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 (Annex 4), 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.

To run TOXSWA create a batch file "`toxswa.bat`" using a text editor in the working folder. The batch file should contain the following line<sup>1</sup>:

```
"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`, the line becomes:

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

The model can be run by running the batch file "`toxswa.bat`" (e.g. by double clicking the file).

---

<sup>1</sup> Note that it is assumed that that TOXSWA is installed in the folder `C:\SWASH\TOXSWA`; if TOXSWA is installed in another folder the path should be adapted likewise.

---

## 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 Section 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 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 at page 56 in Tiktak *et al.* (2000).

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<sup>2</sup>, or prints an error message. If the requested record is found, the model proceeds with

---

<sup>2</sup> Default values are applied for the parameters OptCalcStabilityWater; default = Yes and OptCalcStabilitySediment; default = Yes (see Section 3.3.5), and all print variables; default = No (see Section 3.3.13).

---

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 sediment horizon are allocated to numerical sediment 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,
- Substance<sup>3</sup> properties.

### Numerical records

These records are meant for single numerical values, such as the concentration of suspended solids in water.

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. Note that possible options for the input field are listed here):

```
Transient  OptFloWat    ! Water flow type [Constant, Transient]
```

### 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          ! Starting timeof 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 sediment horizon), and (iii) the obligatory line containing the word 'end\_table'. Comments between the identifier line and the end\_table line are illegal:

```
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
```

---

<sup>3</sup> 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.

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
```

### Substance properties

Values have to be supplied for all substances considered in a simulation run. First, the user has to specify substance 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 substance is added (.e.g. \_PAR, \_MET1 or \_MET2 in the example below).

```
100  DT50WatRef_PAR (d)      ! Half-life transformation in water at reference
                                ! temperature [0.1|1e5]
30   DT50WatRef_MET1 (d)  ! Half-life transformation in water at reference
                                ! temperature [0.1|1e5]
2    DT50WatRef_MET2 (d)  ! Half-life transformation in water at reference
                                ! temperature [0.1|1e5]
```

### 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			Dif	diffusion	Air	air	App	application
Exp	exponent	Area	area	Dis	dispersion	Lay	layer	Avg	average
Fac	factor	Cnt	content	Dra	drainage	Liq	liquid phase	Bal	balance
Fra	fraction	Con	concentration	Drf	drift	Mph	macrophytes	Bas	base
Mol	molar	Del	difference/delta	Ers	erosion	Om	organic matter	Bot	bottom
Nr	number	Dep	depth	Flo	flow	Sed	sediment	Bou	boundary
Num	number	Dst	distance	Flw	flow	Sol	solids	Cha	channel
Tim	time	DT50	transformation time 50%	For	formation	Sus	suspended	Cmp	compound
		Ent	enthalpy	Hyd	hydrology	Sys	water or sediment system	Cre	crest
		Fln	mass flux	Inf	infiltration	Wat	water	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					Del	delete

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

### 3.3.3 Overview of sections in the TOXSWA input file

The TOXSWA input file (`RunId.txw`) 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
0	Run identification	Identification of the run
1	Control	Simulation options
2	Waterbody	Water body properties
3	Hydrology	Hydrology properties
4	Sediment	Sediment properties
5	Weather	Weather properties
6	Temperature	Temperature properties
7	Substance	Substance properties
8	Loadings	Applications, loadings, and catchment factors
9	Initial and boundary conditions for mass balance equations	Initial or boundary concentrations for air, water and sediment
10	Output control	Output options

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

### 3.3.4 Section 0: Run identification

The run identification section contains the composition of the run; identifying which location (`Location`), waterbody (`WaterbodyID`), sediment (`SedimentTypeID`), parent substance (`SubstanceName`) and application scheme (`ApplicationScheme`) have been combined (see Figure 3.1).

```

*-----
*-----
* Section 0: Run identification
*-----

R1_Stream      Location          ! Name of the location [1|25 characters]
R1_Stream      WaterbodyID       ! ID of the water body [1|25 characters]
FOCUS          SedimentTypeID    ! Name of sediment type [1|25 characters]
EXSW2          SubstanceName     ! Name of parent substance [1|15 characters]
EXSW2-maize    ApplicationScheme ! Name of the application scheme [1|25 characters]

```

Figure 3.1 The Identification section in the TOXSWA input file.

### 3.3.5 Section 1: Control

This control section contains general options for the simulation run (see Figure 3.2).

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

FOCUS      CallingProgram      ! Release type of scenario [FOCUS]
5.5.3      CallingProgramVersion ! Version numbers for model, interface and database,
                                         ! respectively

01-Oct-1978 TimStart      ! Starting time of simulation [01-Jan-1900|31-Dec-9999]
30-Sep-1979 TimEnd      ! End time of simulation [01-Jan-1900|31-Dec-9999]

Hourly     OptInp      ! Option for hourly or daily input data of lateral entries [Hourly, Daily]

* OptHyd: options for hydrology simulation
* Only     Simulate only hydrology
* OnLine   Simulate hydrology and substance
* OffLine  Assumption hydrology has been simulated, runID.hyd file must be present
* Automatic TOXSWA checks if hydrology file (runID.hyd) exists; so, hydrology
*          simulation is skipped
Automatic  OptHyd      ! Option selected for hydrology simulation
                                         ! [Only, OnLine, OffLine, Automatic]

600        TimStpHyd (s)  ! Calculation time step for hydrology [0.001|3600]

* OptTem: options for temperature simulation
* Only     Simulate only temperature
* OnLine   Simulate temperature and substance
* OffLine  Assumption temperature has been simulated, runID.tem file must be present
* Automatic TOXSWA checks if the temperature file (runID.tem) exists; so, temperature
*          simulation is skipped
OnLine     OptTem      ! Option selected for temperature simulation
                                         ! [Only, OnLine, OffLine, Automatic, ExtModel]

Calc       OptTimStp ! Option for time step in mass balance calculation [Input, Calc]
Yes        OptCalcStabilityWater ! Option for check of stability of the numerical solution for
                                         ! the water layer
Yes        OptCalcStabilitySediment ! Option for check of stability of the numerical solution for
                                         ! the sediment [Yes, No]
                                         ! Yes = Full check on stability
                                         ! No = Check on positivity

* If OptTimStp is 'Input' then specify
600        TimStpWat (s)  ! Calculation time step in water layer [0.001|3600]
600        TimStpSed (s)  ! Calculation time step in sediment [0.001|3600]

* If OptTimStp is 'Calc' then specify
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]
```

Figure 3.2 The Control section in the TOXSWA input file.

#### Model versions

The model versions are indicated by the variables `CallingProgram` and `CallingProgramVersion`. The `CallingProgram` variable indicates in which context TOXSWA is used (here `FOCUS`), and by `CallingProgramVersion` which version of this context (here `5.5.3`).

#### 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.

#### 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 existing file that was generated in a previous run: a hydrological data file (`RunId.hyd`) and/or a temperature data file (`RunId.tem`).
- `OnLine:` TOXSWA generates the data files.
- `Automatic:` TOXSWA checks if the data file is already available. If so, the

hydrological/temperature calculations will be skipped.  
 Only: The hydrological/temperature module is run, but the remainder of the simulations (i.e. concentrations and mass balances of the substance(s) in the water body) is skipped.

### Simulation time step hydrology

The time step used for the simulation of the hydrology is fixed and set with `TimStpHyd`.

### Simulation time steps and check of stability for mass balance equations

The time step variables are `OptTimStp`, `OptCalcStabilityWater`, `OptCalcStabilitySediment`, `TimStpWat`, `TimStpSed`, `MaxTimStpWat` and `MaxTimStpSed`. The time step for the substance simulations (`OptTimStp`) can be input or calculated by TOXSWA.

The options for check of the stability of the numerical solution can be set with the options `OptCalcStabilityWater` and `OptCalcStabilitySediment`. The default is `Yes` (note that when these parameters are not included in the input file, the default of `Yes` is applied). However, when during a TOXSWA run an error message is given "RDD (or RBD) is not  $\geq 0$ "<sup>4</sup>, then these options can be used to relax the stability criterion, to circumvent the run to stop. Note that when this option is applied, we suggest to check the plausibility of the calculated concentration profile, e.g. no unrealistic oscillations may occur.

When the option `Input` is used the time step for water (`TimStpWat`) and for sediment (`TimStpSed`) can be entered. When the option `Calculated` (`Calc`) is used the maximum time step for water (`MaxTimStpWat`) and for sediment (`MaxTimStpSed`) can be entered. For FOCUS simulations the option `Calculated` (`Calc`) is used.

## 3.3.6 Section 2: Water body

The Water body section specifies the dimensions of the water body and the characteristics of the water layer (see Figure 3.3).

### Name and ID

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

```

*-----
*-----
* Section 2: Waterbody
*-----
* WaterBody table: description of waterbody
* Len          Length [0.05]
* NumSeg       Number of segments [1]
* WidWatSys    Width of the bottom of water system [0.05|100]
* SloSidWatSys Side slope of the water system [0|10]
* DepWatDefPer Water depth defining perimeter for exchange between water layer
*              and sediment [0|lowest water depth]
table WaterBody
Len  NumSeg  WidWatSys  SloSidWatSys  DepWatDefPer
(m)  (-)      (m)         (-)           (m)
100  20       1           1.E-5         0.01
end_table

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

```

Figure 3.3 The Water body section in the TOXSWA input file.

<sup>4</sup> Example of error message, given for water layer and RDD not  $\geq 0$ :

RDD for water layer  $< 0$ , so the numerical solution of the mass balance equation for the water layer may result in negative or unstable concentrations; This occurs in water layer segment: 2 at time 30-Oct-1992-00h30 using time step 7.407 s.

Options to solve this are: 1. Relax the stability criterion for the numerical solution and check only on positive concentrations, or 2. Rerun the simulation for a smaller time step for the water layer than the one reported above, e.g. by dividing the reported time step by 2 (iteratively). For option 1 we suggest to check the plausibility of the calculated concentration profile, e.g. no unrealistic oscillations may occur. Option 2 has the disadvantage of a longer run time for TOXSWA.

## 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 12 in Ter Horst *et al.*, 2016).

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 the 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 Ter Horst *et al.*, 2016). 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.twx` 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 m<sup>2</sup> water body bottom (`AmaMphWatLay`) have to be entered.

### 3.3.7 Section 3: Hydrology

The Hydrology section specifies the type of hydrology of the water body, and the parameterisation of the selected hydrology type. The section consists of a general section (Section 3a) in which the type of hydrology is specified and three individual sections for each type of hydrology (Sections 3b – 3d) (see Figure 3.4). 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 *et al.* (2017), Ter Horst *et al.*, (2016), and in Adriaanse and Beltman (2009).

#### Section 3a: Definition of water flow, water body type and dispersion

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

In waterbodies consisting of one segment in the water layer (ponds) longitudinal dispersion is not calculated. For watercourses this type of dispersion is taken into account. The option `OptDis` indicates using an input value, or calculating the dispersion coefficient according to Fischer (see Annex 6). When the option `Input` is selected a value for the dispersion coefficient must be entered (`CofDisPhsInp`).

TOXSWA uses only those parameters in Sections 3b - 3d that concern the selected options in Section 3a for type of water flow and type of waterbody (`OptFloWat`, `OptWaterSystemType`) (see Table below). The parameters in the sections not relevant for the chosen options will not be used by TOXSWA.

Section	OptFloWat		OptWaterSystemType	
	Constant	Transient	Pond	WaterCourse
<i>3b: Constant flow</i>	x		x	x
<i>Section 3c: Variable flow in a pond</i>		x	x	
<i>Section 3d: Variable flow in a watercourse</i>		x		x

### Section 3b: Constant flow

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.

### Section 3c: Variable flow in a pond ( )

The area around the pond that contributes water and pesticide fluxes to the pond is defined by AreaSurPndInp. The fluxes in the drainage or runoff files (indicated in Section 8 in the input file) 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. If runoff is the selected lateral entry route the area AreaErsSurPndInp contributes pesticide fluxes by erosion.

### Section 3d: Variable flow in a watercourse

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.

```
*-----
*
* Section 3: Hydrology:
*   Section 3a: General
*-----

Transient   OptFloWat           ! Water flow type [Constant, Transient]
WaterCourse OptWaterSystemType ! Water system type [Pond, WaterCourse]

* If OptWaterSystemType is 'WaterCourse' then specify
Fischer     OptDis              ! Dispersion calculation method [Input, Fischer]

* If OptDis is 'Input' then specify
600         CofDisPhsInp (m2.d-1) ! Dispersion coefficient [0|1e6]

*-----
* Section 3b: Constant water flow
*
* If OptFloWat is 'Constant'
*-----

1           DepWat (m)           ! Water depth [0.001|10]
100        VelWatFlwBas (m.d-1) ! Flow velocity [-1e5|1e5]

*-----
* Section 3c: Variable flow: pond
*
* If OptFloWat is 'Transient' and OptWaterSystemType is 'Pond'
*-----

0.45       AreaSurPndInp (ha ) ! Size of surrounding area discharging excss water into the pond
! [0|100]
3.189      QBasPndInp (m3.d-1) ! Base flow, i.e. inflow into pond [0|50]
0.5        HgtCrePnd (m)       ! Height of the weir crest at outflow [0.1|5]
0.5        WidCrePnd (m)       ! Width of the weir crest at outflow [0.01|10]

* If application option OptLoa is 'PRZM' then specify
0.06       AreaErsSurPndInp (ha) ! Size of the eroding area around the pond [0|100]

*-----
* Section 3d: Variable flow: watercourse
*
* If OptFloWat is 'Transient' and OptWaterSystemType is 'WaterCourse'
*-----

100        AreaUpsWatCrSInp (ha) ! Area of upstream catchment [0|1e4]
191.8      QBasWatCrSInp (m3.d-1) ! Base flow from upstream catchment [0|1e4]
0.001      SloBotRepCha (-)      ! Slope bottom representative channel [0|0.01]
0.5        HgtCreRepCha (m)      ! Height of the weir crest [0.01|5]
0.5        WidCreRepCha (m)      ! Width of the weir crest [0.01|10]
110        LenRepCha (m)         ! Length representative channel [10|2000]
11         CofRghRef (s-1)       ! Value Manning coefficient for bottom roughness at 1 m
! water depth in water body [1|100]
1.2        CofVelHea (m.s-1)     ! Energy coefficient due to non-uniform distribution of
! flow velocities in cross section [1.1|1.5]
```

Figure 3.4 The Hydrology section in the TOXSWA input file.

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,  $QBasRepChaInp$ , and either the runoff or the drainage fluxes from the upstream catchment with area  $AreaUpStrRepChaInp$ . 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.

### 3.3.8 Section 4: Sediment

In this section, the sediment profile, vertical discretization and sediment properties have to be specified (see Figure 3.5).

#### Sediment profile

The vertical discretization of the sediment 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 layer thickness is taken too large. Furthermore, then mass balance errors may become too large. For most simulations, however, a layer 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 ( $\varepsilon$ ,  $ThetaSat$ ) from the dry bulk density ( $\rho_d$ ,  $Rho$ ), the phase densities of organic matter ( $\rho_{om}$  in  $kg\ L^{-1}$ ) and of mineral matter ( $\rho_{min}$  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  $\rho_{om}$  and  $2.65\ kg\ L^{-1}$  for  $\rho_{min}$  (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 ( $\lambda$ ,  $CofDifRel$ ) 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<sup>5</sup> (`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.

### 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.

```

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

* SedimentProfile table: thickness and number of layers in horizon
* ThiHor Thickness of horizon [0.0001|-]
* NumLay Number of layers in horizon [1|500]
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 ! Sediment properties for ThetaSat and CofDifRel [Input, Calc]

* SedimentProperties table: properties for each horizon:
* Nr Number horizon [1|500]
* Rho Bulk density [10|3000]
* CntOm Organic matter mass content [0|1]
* If OptSedProperties 'Input' then specify ThetaSat and CofDifRel
* ThetaSat Saturated water content [0.001|0.999]
* CofDifRel Relative diffusion coefficient [0|1]
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) ! Percolation rate through the sediment [-0.01|0.01]

* DispersionLength table: dispersion length for each horizon
* Nr Horizon number [1|500]
* LenDisSedLiq Dispersion length of solute in liquid phase (m) [0.01|1]
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

```

Figure 3.5 The Sediment section in the TOXSWA input file.

<sup>5</sup> The relative diffusion coefficient is also called tortuosity.

---

### 3.3.9 Section 5: Weather

The Weather section specifies weather data (see Figure 3.6). 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. `Monthly` needs to be indicated (`OptMetInp`).

```
*-----  
*-----  
* Section 5: Weather  
*-----  
  
Weiherbach   MeteoStation   ! Name of file with meteo data (*.met)  
Monthly      OptMetInp      ! Input data [Monthly]
```

Figure 3.6 The Weather section in the TOXSWA input file.

Note that the input of Section 6 Temperature is not needed for TOXSWA kernel 3.3.6 in FOCUS\_TOXSWA 5.5.3. The module for calculating hourly/daily water temperatures is not yet operational in TOXSWA kernel 3.3.6. Its corresponding input section (Section 6 in the input file) in the TOXSWA input file is therefore not described in this report.

### 3.3.10 Section 7: Substance properties

The Substance section lists the properties of all substances (see Figure 3.7). The Substance section consists of a general part (Section 7a) followed by a separate section for each substance (Sections 7b etc.). In this section of the TOXSWA input file, the identifier names are concatenated with substance names (in this example EXSW2). The maximum length of each code is 15 characters.

#### Section 7a: Compounds and metabolite schemes

A list of substance codes of all substances in the simulation<sup>6</sup> should be entered in the `table compounds`.

The transformation scheme for substances formed in water (see also Figure 3.7) is input in the `table FraPrtDauWat`. For each parent substance, the molar fraction of substance transformed into a daughter must be specified. Figure 3.7 shows an example for three transformations; the parent substance EXSW2 is for 70% transformed into the daughter METW1. This daughter METW1 is for 100% transformed into a consecutive daughter METW2. Next to the parent also a metabolite formed in soil METSO enters the water body, which is for 50% transformed into *daughter* METW2. For transformations in sediment the substances and formation fractions must be entered similarly in `table FraPrtDauSed`.

For each substance simulated a section needs to be prepared. Hence, in the example next to Section 7b for the parent EXSW2, Sections 7c – 7e for the metabolites METW1, METW2 and METSO must be prepared (Note that Sections 7c – 7e for these metabolites are not shown in Figure 3.7).

---

<sup>6</sup> In this manual the parent EXSW2 is used to illustrate input and output of TOXSWA. EXSW2 has no metabolites. When metabolite options needed be illustrated the following metabolites are used: METW1; metabolite formed in water from parent EXSW2; METW2, metabolite formed in water from metabolite METW1, METSO; metabolite formed in soil from parent EXSW2.

```

-----
*
* Section 7: Substance
* Section 7a: general
-----

* Compounds table: first entry is parent, next e+tries are metabolites [1|15 characters]
table compounds
EXSW2
METW1
METW2
METS0
end_table

* FraPrtDauWat table: parent-daughter relationships transformation in water
* Column 1: fraction formed from parent into daughter [0|]
* Column 2: name of parent
* Column 3: name of daughter
table FraPrtDauWat (mol.mol-1)
0.7 EXSW2 -> METW1
1 METW1 -> METW2
0.5 METS0 -> METW2
end_table

* FraPrtDauSed table: parent-daughter relationships transformation in sediment
* Column 1: fraction formed from parent into daughter [0|]
* Column 2: name of parent
* Column 3: name of daughter
table FraPrtDauSed (mol.mol-1)
end_table

-----
* Section 7b: Substance properties for parent 'SubA'
* (note extension of parameter name is substance code)
-----

300 MolMas_EXSW2 (g.mol-1) ! Molar mass [10|10000]

* Volatilization from water layer
1.E-4 PreVapRef_EXSW2 (Pa) ! Saturated vapour pressure of substance [0|2e5]
20 TemRefVap_EXSW2 (C) ! Reference temperature for saturated vapour pressure
! [0|40]
95. MolEntVap_EXSW2 (kJ.mol-1) ! Molar enthalpy of vaporization [-200|200]
1 SlbWatRef_EXSW2 (mg.L-1) ! Water solubility of substance [0.001|1e6]
20 TemRefSlb_EXSW2 (C) ! Reference temperature for water solubility [0|40]
27 MolEntSlb_EXSW2 (kJ.mol-1) ! Molar enthalpy of dissolution [-200|200]

* Diffusion in liquid phase
4.3E-5 CofDifWatRef_EXSW2 (m2.d-1) ! Reference diffusion coefficient in water [0|2E-3]

* Sorption
58 KomSed_EXSW2 (L.kg-1) ! Freundlich coefficient of equilibrium sorption for
! sediment [0|1e7]
1 ConLiqRefSed_EXSW2 (mg.L-1) ! Reference concentration in liquid phase for
! Freundlich coefficient for sediment [0.001|100]
1 ExpFreSed_EXSW2 (-) ! Freundlich exponent in sediment [0.1|1.5]
58 KomSusSol_EXSW2 (L.kg-1) ! Freundlich coefficient of equilibrium sorption
! for suspended solids [0|1e7]
1 ConLiqRefSusSol_EXSW2 (mg.L-1) ! Reference concentration in liquid phase
! for Freundlich sorption coefficient for
! suspended solids [0.001|100]
1 ExpFreSusSol_EXSW2 (-) ! Freundlich exponent suspended solids [0.1|1.5]
0 CofSorMph_EXSW2 (L.kg-1) ! Coefficient for linear sorption on
! macrophytes [0|1e7]

* Transformation in water
2 DT50WatRef_EXSW2 (d) ! Half-life transformation in water at reference
! temperature [0.1|1e5]
20 TemRefTraWat_EXSW2 (C) ! Reference temperature for half-life measured in
! water [5|30]
65.4 MolEntTraWat_EXSW2 (kJ.mol-1) ! Molar activation enthalpy of transformation in
! water [0|200]

* Transformation in sediment
3 DT50SedRef_EXSW2 (d) ! Half-life transformation in sediment at reference
! temperature [0.1|1e5]
20 TemRefTraSed_EXSW2 (C) ! Reference temperature for half-life in sediment
! [5|30]
65.4 MolEntTraSed_EXSW2 (kJ.mol-1) ! Molar activation enthalpy of transformation in
! sediment [0|200]

```

Figure 3.7 The Substance section in the TOXSWA input file.

---

## Section 7b: Substance properties for substance

### *Molar mass*

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

### *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 substance property and must be specified in this section. The relative diffusion coefficient is specified in the sediment section (Section 3.3.7).

### *Sorption*

The sorption of substances 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<sup>-1</sup>. 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.

### *Transformation in water*

The DegT50 of the substance 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).

### *Transformation in sediment*

The DegT50 of the substance in the sediment (`DT50SedRef`) and the temperature at which it is measured (`TemRefTraSed`) have to be entered. The molar activation enthalpy (`MolEntTraSed`) 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).

## 3.3.11 Section 8: Loadings

The Loadings section concerns loadings (spray drift, drainage, and runoff) into the water body, and upstream catchment options relevant for the loadings (see Figure 3.8).

### **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.

### **Loadings table: 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.twx` 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

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`. 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.

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 containing the runoff or drainage fluxes of the metabolite need to be specified in this table as well. For each substance (parent and its soil metabolites) a separate file with drainage or runoff fluxes is needed.

### 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

In the upstream catchment of FOCUS stream scenarios metabolites are formed in molar fractions varying between 0 (no metabolite formation) and 1 (1 mol parent has been transformed into 1 mol metabolite). A factor,  $CF_{m,up}$  (`FraMetForUps`), is needed to account for this. This correction factor is specific for the metabolite, the parent substance and the scenario (because of the temperature as well as the time spent in the upstream catchment during which the metabolite can be formed). The correction factor accounts both for metabolite mass formed from parent mass deposited by spray drift on the water surface area in the upstream catchment, and for metabolite mass formed from parent mass originated from drainage or runoff in the upstream catchment. See Adriaanse *et al.* (2014) for the theoretical basis of this correction factor and the procedure to calculate it. Because these correction factors depend on the substance as well as the scenario they have been incorporated in the loadings section of the input file; see Figure 3.8. Note that the name of the substance (`METW1`) is incorporated in the parameter name, because the parameter is substance specific. Furthermore, correction factors are not given for metabolites `METW2` and `METSO` (see Figure 3.7), because these are not primary metabolites formed in water from the parent substance.

```

-----
-----
* Section 8: Loadings
*
-----

* OptLoa options for loading type
* DriftOnly spray drift only entry route
* MACRO drainage calculated by MACRO
* PRZM runoff and erosion calculated by PRZM
MACRO OptLoa ! Loading option [DriftOnly, PEARL, MACRO, PRZM, GEM]

* Loadings table: details on spray drift, and stretch for all loading types
* Column 1 Date and time of application, relevant if OptLoa is 'DriftOnly', otherwise
* the date is a dummy value
* Column 2 Type of loading [Drift]
* Column 3 Drift deposition (mg.m-2) [0|]
* Column 4 Start of stretch of watercourse loaded by all loading types (m) [0|1e4]
* Column 5 End of stretch of watercourse loaded by all loading types (m) [0|1e4]
table Loadings
30-Dec-1899 drift 1.5400E-001 0. 30.
30-Dec-1899 drift 1.1550E-001 0. 30.
30-Dec-1899 drift 7.7000E-002 0. 30.
end_table

* If OptLoa is 'MACRO' then specify details of drainage
0. WidFldDra (m) ! Width of field contributing drainage

* If OptLoa is 'PRZM' then specify details of runoff
100 WidFldRnf (m) ! Width of field contributing runoff [0|1000]
20 WidFldErs (m) ! Width of field contributing erosion [0|1000]
0 RatInfDir (-) ! Ratio of infiltration water added to runoff water [0|1]
0.01 ThiLayErs (m) ! Thickness of upper sediment layer to which erosion mass
! is added [1e-5|1]

* If OptLoa is 'MACRO' or OptLoa is 'PRZM' then specify path and file names of files
* Table lateral entries files of soil substances, including metabolites (path+name)

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

* If OptHyd is 'transient' then specify details of catchment
Yes OptUpsInp ! Upstream catchment treated [Yes, No]
0.2 RatAreaUpsApp (-) ! Ratio of upstream catchment treated [0|1].

.

* If metabolite formed in water then
0.013 FraMetForUps_METW1 (-) ! Fraction metabolite formed in water in
! upstream catchment [0|1]

```

Figure 3.8 The Loadings section in the TOXSWA input file.

### 3.3.12 Section 9: Initial and boundary conditions for mass balance equations

The Initial and boundary conditions section concerns initial and boundary concentrations for air, water, sediment and seepage (see Figure 3.9).

#### 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 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.

#### 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 3.3.4) and the seepage is upward in the water body (negative values) the concentration in incoming seepage water (ConWatSpg) can be specified.

```
*-----
*-----
* Section 9: Initial and boundary conditions for mass balance equations
*
*-----
* Initial conditions
0          ConSysWatIni (g.m-3) ! Initial total concentration in water layer [0|-]
* CntSysSedIni table: initial total substance content in sediment
* If metabolites are included then initial contents for these substances are set to zero
* Column 1 Depth in sediment (m) [0|-]
* Column 2 Substance content (mg.kg-1) [0|-]
table interpolate CntSysSedIni (mg.kg-1)
end_table
* Boundary conditions
0          ConAir (g.m-3)      ! Concentration in air [0|-]
0          ConWatSpg (g.m-3)   ! Concentration in incoming seepage water [0|-]
```

Figure 3.9 The Initial and boundary section in the TOXSWA input file.

### 3.3.13 Section 10: Output control

In this section, the output of TOXSWA is controlled. The Output control section consists of three parts; Section 10a for general settings (see Figure 3.10), Section 10b for additional options for Dutch registration reports (not described here), and Section 10c to specify which variables are selected to print in the output file (see Figure 3.11).

#### Section 10a: General settings

##### 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.

##### 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.

##### Output time step

With `OptDelTimPrn` the output time step is set. The following options are available: `Hour`, `Day`, `Decade`, `Month`, `Year`, `Automatic` and `Other`. If `OptDelTimPrn` is `Other`, the time step is set with `DelTimPrn`.. If set to zero, TOXSWA will calculate the output interval based on begin and end date of the simulation. It is important to realise 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)..

```

*-----
*-----
* Section 10: Output control
*   Section 10a: General
*-----

No      OptDelOutFiles  ! Remove *.out file after simulation [Yes|No]

* DateFormat: options for format of date and time in the output file
* DaysFromSta  Print number of days since start of simulation
* DaysFrom1900 Print number of days since 1900
* Years        Print years
DaysFromSta DateFormat [DaysFromSta, DaysFrom1900, Years]

* RealFormat: format of the ordinary output - use FORTRAN notation:
* e is scientific notation, g is general notation,
* then the number of positions, then the number of digits
e14.6      RealFormat      ! Format of ordinary output

* OptDelTimPrn: options for output time step
* Hour,Day,Decade,Month,Year  Time step for output
* Automatic                    Length of simulation period
* Other                         User defined
Hour      OptDelTimPrn      ! Output time step [Hour|Day|Decade|Month|Year|
! Automatic|Other]

* If OptDelTimPrn is 'Other' then specify
5         DelTimPrn (d)      ! Output time step [1|length simulation period]
! Integer value required

0.05     ThiLayTgt (m)      ! Depth defining the thickness of the target sediment layer
! for output of (averaged) content [1e-5|1]

table    OptOutputDistances ! Options for distances of water layer grid points at which
! output can be obtained[None, All, table]

* If OptOutputDistances is 'table' then specify output distances in waterbody
* OutputDistances-table: output distances in waterbody, i.e. water layer and sediment
* subsystem
* Column 1 Distance (m) [0|-]
table OutputDistances (m)
97.5
end_table

table    OptOutputDepths   ! Options for depths of sediment grid points at which
! output can be obtained [None, All, table]

* If OptOutputDepths is 'table' then specify
* OutputDepths-table: depths of sediment nodes at which output can be obtained
* Column 1 Depth (m) [0|-]
table OutputDepths (m)
0.003
horizont 0.05
end_table

* Specify dates for output of additional profiles; options set via OptOutputDistances and
* OptOutputDepths are used
* HorVertProfiles table: profiles in horizontal direction for water layer and in vertical
* direction for sediment are given; values given are:
* Water layer: output distance, water depth, total and dissolved concentration,
* Sediment: output node water layer, output depth, pore volume, total and dissolved
* concentration.
table HorVertProfiles
03-Jan-1979-0000end_table

* Specify type of summary report
FOCUS    OptReport        ! [FOCUS]
Yes      ExposureReport   ! Exposure report [Yes|No]

```

Figure 3.10 The Output control section in the TOXSWA input file; Section 10a General settings

### 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.

### Distances and depths

An option for the output of the variables in the water layer (`OptOutputDistances`) must be selected. If the option `None` is selected, no values for the individual water segments are given in the output, or if the option `All` is selected, values for all segments in the water layer are given. If the option `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.

```

-----
* Section 10c: Print variables in *.out file
* State variables, fluxes and rates given as momentary values.
* Volume,energy and mass changes given as cumulative values.
-----

* Specify for all print variables whether output is wanted [Yes, No]
* When print variable is not in file; TOXSWA assumes 'No'

* PrintCumulatives: options for printing cumulatives of volume, energy and mass fluxes
* Yes : cumulative terms have been summed up from start of simulation and have been
*       allocated to the last moment of the period considered
* No  : cumulative terms have been summed up from start of user defined output time step
*       OptDelTimPrn and have been allocated to the last moment of the period
*       considered
Yes   PrintCumulatives      ! [Yes, No]

* Hydrology
Yes   print_DepWat          ! Water depth (m)
Yes   print_QBou            ! Discharge (m3.s-1)
Yes   print_VelWatFlw      ! Flow velocity (m.d-1)
Yes   print_VolErrWatLay   ! Volume error in waterbody (m3)

* Lateral entries (expressed per m2 adjacent field)
* If OptLoa is 'MACRO'
Yes   print_VvrLiqDra      ! Drain flow (m3.m-2.hr-1)
Yes   print_FlmDra        ! Drain substance flux (g.m-2.hr-1)
* If OptLoa is 'PRZM'
Yes   print_VvrLiqRnf     ! Runoff (+ infiltration) water flow (m3.m-2.hr-1)
Yes   print_FlmRnf        ! Runoff substance flux (g.m-2.hr-1)
Yes   print_FlmErs        ! Erosion substance flux (g.m-2.hr-1)

* Concentrations and contents in water layer segments as specified by
* OptOutputDistances
Yes   print_ConLiqWatLay   ! Concentration dissolved in water (g.m-3)
No    print_CntSorMph      ! Content sorbed to macrophytes (g.kg-1)
No    print_CntSorSusSol   ! Content sorbed to suspended solids (g.kg-1)
No    print_ConSysWatLay   ! Total concentration in water (g.m-3)

* Concentrations and contents in sediment below water layer segments as specified by
* OptOutputDistances and OptOutputDepths
Yes   print_ConLiqSed      ! Concentration in pore water sediment (g.m-3)
No    print_CntSorSed     ! Content sorbed to sediment (g.kg-1)
No    print_ConSysSed     ! Total content in sediment (g.m-3)
No    print_CntSedTgt     ! Total content in target layer sediment (g.kg-1)
Yes   print_ConLiqSedTgt  ! Concentration in pore water in target layer
! sediment (g.m-3)
No    print_CntSorSedTgt  ! Content sorbed in target layer sediment (g.kg-1)

* Distribution in entire water layer
Yes   print_MasLiqWatLay   ! Mass in liquid phase in water layer (g)
Yes   print_MasSorSusSol   ! Mass sorbed to suspended solids in water layer (g)
Yes   print_MasSorMph      ! Mass sorbed to macrophytes in water layer (g)

* Distribution in entire sediment
Yes   print_MasLiqSed     ! Mass in liquid phase in sediment (g)
Yes   print_MasSorSed     ! Mass sorbed in sediment (g)

* Mass balance for entire water layer
Yes   print_MasWatLay     ! Mass in water layer (g)
Yes   print_MasDrfWatLay  ! Mass entered in water layer by spray drift (g)
Yes   print_MasDraWatLay  ! Mass entered in water layer by drainage (g)
Yes   print_MasRnfWatLay  ! Mass entered in water layer by runoff (g)
Yes   print_MasSedInWatLay ! Mass penetrated into sediment from water layer (g)
Yes   print_MasSedOutWatLay ! Mass transferred from sediment into water layer (g)
Yes   print_MasDwnWatLay  ! Mass flowed across downstream boundary out of
! water layer (g)
Yes   print_MasUpsWatLay  ! Mass flowed across upstream boundary into water
! layer (g)
Yes   print_MasTraWatLay  ! Mass transformed in water layer (g)
Yes   print_MasForWatLay  ! Mass formed in water layer (g)
Yes   print_MasVolWatLay  ! Mass volatilised from water layer (g)
Yes   print_MasErrWatLay  ! Mass error in water layer (g)

* Mass balance sediment
Yes   print_MasSed        ! Mass in sediment (g)
Yes   print_MasTraSed     ! Mass transformed in sediment (g)
Yes   print_MasForSed     ! Mass formed in sediment (g)
Yes   print_MasWatLayInSed ! Mass transferred into water layer from sediment
! layer (g)
Yes   print_MasWatLayOutSed ! Mass transferred from water layer into sediment
! layer (g)
Yes   print_MasDwnSed     ! Mass leaving sediment across lower boundary (g)
Yes   print_MasErsSed     ! Mass entering sediment by erosion (g)
Yes   print_MasErrSed     ! Mass error in sediment (g)

```

Figure 3.11 The Output control section in the TOXSWA input file; Section 10c Print variables in output file. Note that the input file uses the term "Mas" in mass balance parameters. However, in the graphs part of the user interface of FOCUS\_TOXSWA 5.5.3 the old term "Ama" is still used (has not effect on usage or results)

---

An option for the output of the variables in the sediment (`OptOutputDepths`) must be selected. If the option `None` is selected, no values for the individual sediment layers are given in the output, or if the option `All` is selected, values for all layers in the sediment are given. If the option `table` is selected, In the `table OutputDepths` it can be specified for which depths in the sediment output is requested. Then the output for the middle of the layer that is closest to the requested depth is given. Output as function of distance in the water layer and/or as a function of depth in the sediment is produced only at the dates specified in the `HorVertProfiles` table.

#### *Horizontal profiles in water layer and vertical profiles in sediment*

The user can specify a number of dates at which horizontal profiles of the most important state variables in the water layer, and vertical profiles of the most important state variables in the sediment are produced (`table HorVertProfiles`). The segments in the water layer for which sediment layer values are given are set via the option `OptOutputDistances`.

#### *Type of summary report*

The type of summary report needed from the run is specified (`OptReport`), and it can be set whether the summary report (see Section 3.10) should include the exposure report (`ExposureReport`).

**Section 10b Additional options for the Dutch registration report is not described here, because it is not relevant for FOCUS\_TOXSWA 5.5.3.**

### **Section 10c: Print variables in output file**

#### *Print cumulatives*

With `PrintCumulatives` it is indicated if volume, energy and mass fluxes in the output must be given as cumulative of the output time step (`No`) or accumulated during the simulation (`Yes`). For the accumulation two options are available via the parameter `PrintCumulativesSta`; i) `Yes`; the values are accumulated from the start of the simulation, or ii) `No`; the values are accumulated after the initialisation period (warming up period) was ended.

#### *Print variables*

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

Note that the following is applicable if `PrintCumulatives` is set to `No`: For the volume, energy and mass fluxes of which the output is given as e.g.  $\text{m}^3$  of g, the value is per output time step, e.g. when `Mass transformed in water layer` is 5, and the output time step is 1 hour, then the transformed mass is 5 g in the past hour. However if the option `PrintCumulatives` is set to `Yes`; the mass is the cumulative mass during the simulation, or since the end of the initialisation period (see the section on `PrintCumulatives` for more details). I.e. the volume, energy and mass fluxes are either given as cumulative of the output time step or as cumulative of the simulation period

## 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 3.12.

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

```

*
* 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 3.12 Example of a meteo input file.

### 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 3.13. In the header the dates of the applications and corresponding application rates are indicated. TOXSWA reads the dates of the applications and allocates them to the timings of the spray drift events.

The **RunId.p2t** file is an output file of the PRZM model containing the hourly runoff water and pesticide fluxes as well as the hourly eroded soil and pesticide fluxes (sorbed onto the eroded soil) entering the water body by runoff and associated erosion. An example of a **RunId.p2t** file is shown in Figure 3.14. The last column lists the infiltration below 1 m depth. In the header the dates of the applications and corresponding application rates are indicated. TOXSWA reads the dates of applications and allocates them to the timings of the spray drift events.

```

* MACRO to TOXSWA input file (C:\SwashProjects\project_EXSW2\MACRO\cereals_winter\
macro00001_p.m2t) created on 06/12/2017 09:55:05
*
* MACRO in FOCUS Version 5.5.4
* Output File = C:\SwashProjects\project_EXSW2\MACRO\cereals_winter\macro003.bin
* Type of compound = parent
* Run ID = 165
* Compound : EXSW2
* Scenario : D4
* Surface water (drained at 1.2 m depth and 10 m spacing)
*
* Simulation from 19790101 to 19860501, 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 3.13 The MACRO output file containing hourly water and pesticide fluxes, entering the water body by drainage for TOXSWA.

```

*-----
* TOXSWA REPORT: Water and mass balances

* Table: Water balance of the water body
* 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 100.00 m
*-----
* Year Month Identifier      DelSto      VolPrc      VolDra      VolRun      VolUps      VolDwn
*-----
1978 Oct BalWatLay          -0.0050    0.0000    0.0000    0.0000    8011.9925    8039.6526
1978 Nov BalWatLay           0.0610    0.0000    0.0000    0.0000    7292.0580    7309.1270
1978 Dec BalWatLay           1.7490    0.0000    0.0000    0.0000    23593.1331    23785.6926
1979 Jan BalWatLay          -1.4610    0.0000    0.0000    0.0000    8557.3991    8584.9932
1979 Feb BalWatLay           1.0370    0.0000    0.0000    0.0000    15313.7603    15425.8857
1979 Mar BalWatLay          -0.5170    0.0000    0.0000    0.0000    11458.2459    11514.3887
1979 Apr BalWatLay          -0.6550    0.0000    0.0000    0.0000    10631.5874    10690.9822
1979 May BalWatLay          -0.2540    0.0000    0.0000    0.0000     6658.4739     6665.9724
1979 Jun BalWatLay          -0.1550    0.0000    0.0000    0.0000     5754.4327     5754.5939
1979 Jul BalWatLay           0.0000    0.0000    0.0000    0.0000     5945.7802     5945.7802
1979 Aug BalWatLay           0.0000    0.0000    0.0000    0.0000     7587.2830     7612.3190
1979 Sep BalWatLay           0.0000    0.0000    0.0000    0.0000     5756.9530     5756.9821
*-----

* Annual water balance terms (m3) in water system of 100.00 m
* (year may be incomplete)
*-----
* Year Identifier      DelSto      VolPrc      VolDra      VolRun      VolUps      VolDwn
*-----
1978 BalWatLay          1.8050    0.0000    0.0000    0.0000    38897.1836    39134.4722
1979 BalWatLay          -2.0050    0.0000    0.0000    0.0000    77663.9154    77951.8974
*-----

```

Figure 3.14 The PRZM output file containing hourly water and pesticide fluxes, entering the water body by runoff and erosion for TOXSWA

### 3.6 The summary output file

The summary output file has the extension .sum (RunId.sum). It gives the main inputs and a summary of the output, i.e. water and mass balances, and the target concentrations (Figure 3.15a-f).

The header of the file presents information about the performed run. Information is given about the model versions used for the executed run. Therefore, it can always be traced back with which model versions the results were obtained. The 8<sup>th</sup> line gives the folder on your PC where the simulation was performed. The date on the 10<sup>th</sup> line of the header indicates the date that the simulation was performed. The shells of SWASH and of TOXSWA automatically assign an ID number to a run.

#### 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 4.4.5). The maximum hourly fluxes and the maximum hourly concentrations in drained water or runoff from the entries are given.

```

* -----
* TOXSWA REPORT: Header

* Results from the TOXSWA model (c) Wageningen University & Research
* FOCUS TOXSWA version : 5.5.3
* TOXSWA model version : 3.3.6
* TOXSWA created on : 17-Dec-2017

* Working directory : C:\SwashProjects\Project_1\TOXSWA
* Run ID : 3
* Input file generated on : 25-09-2018
* -----

* Scenario : R1_Stream
* Meteo Station : Weiherbach
* Substance : EXSW2
* Flow Type : Transient
* Water Body Type : R1_STREAM
* Application Scheme : FOCUS_EXAMPLE
* Simulation Period : 01-Oct-1978 to 30-Sep-1979
* -----
* 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, lumped (d): 100.00 at reference temperature (C) : 20.0
* Half-life in sediment (d) : 300.00 at reference temperature (C) : 20.0
* Kom susp.solids (Freundlich coef. for sorption on organic matter) (L.kg-1) : 58.00
* Freundlich exponent (-) : 1.00
* Kom sediment (Freundlich 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 14-Nov-1978-09h00 1000.0000 1.7160

* Lateral entries: runoff and erosion Simulated by: PRZM

* Maximum hourly fluxes from lateral entries
* Year Type Water/Substance Flux Date
  1978 Water 0.4127 mm.m-2.hr-1 31-Dec-1978-00h30
  1978 Runoff EXSW2 0.01226 mg.m-2.hr-1 25-Nov-1978-00h30
  1978 Runoff EXSW2 215.6 ug.L-1 25-Nov-1978-00h30
  1978 Erosion EXSW2 0.000007 mg.m-2.hr-1 25-Nov-1978-00h30
  1979 Water 0.3578 mm.m-2.hr-1 02-Feb-1979-00h30
  1979 Runoff EXSW2 < 1e-6 mg.m-2.hr-1 02-Feb-1979-00h30
  1979 Runoff EXSW2 0.000051 ug.L-1 02-Feb-1979-00h30
  1979 Erosion EXSW2 < 1e-6 mg.m-2.hr-1 02-Feb-1979-00h30
*
* End of TOXSWA REPORT: Substance properties and substance loadings
* -----

```

Figure 3.15a The summary output file: substance properties and substance loadings

### Water balance

The elements of the water balance are given in a table with monthly values and in a table with annual values (see Figure 3.15b). Note that when only part of the year is simulated, the yearly balance only considers this part of the year.



```

* Table: Mass balance of substance in the water layer
* Key to the table
* -----
* DelMas      Change in mass present in water layer system (g)
* MasIni      Mass initially present in water layer (g)
* MasDrf      Loading of water body by drift (g)
* MasAtmDep   Loading of water body by atmospheric deposition (g)
* MasDra      Loading of water body by drainage (g)
* MasRnf      Loading of water body by run-off (g)
* MasSedIn    Mass penetrated into sediment (g)
* MasSedOut   Mass transferred out of sediment (g)
* MasDwn      Mass flowed across downstream boundary end (g)
* MasUps      Mass flowed across upstream boundary (g)
* MasTra      Mass transformed in water layer (g)
* MasFor      Mass formed in water layer (g)
* MasVol      Mass volatilised from water layer (g)
* -----
*
* -----
* Monthly mass balance terms (g) in entire water layer of water body system of 100.00 m for substance: EXSW2
* Year  Month  DelMas  MasIni  MasDrf  MasAtmDep  MasDra  MasRnf  MasSedIn  MasSedOut  MasDwn  MasUps  MasTra  MasFor  MasVol
* -----
1978  Oct    0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
1978  Nov    0.0000  0.0000  0.1716  0.0000  0.0000  0.0000  0.8582  -0.0211  0.0180  -18.1896  17.1640  -0.0011  0.0000  -0.0000
1978  Dec   -0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0083  -0.0004  0.0022  -0.1763  0.1662  -0.0000  0.0000  -0.0000
1979  Jan   -0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0003  -0.0003  0.0000  -0.0000  0.0000  -0.0000
1979  Feb   -0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0001  -0.0002  0.0000  -0.0000  0.0000  -0.0000
1979  Mar   -0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0001  -0.0001  0.0000  -0.0000  0.0000  -0.0000
1979  Apr    0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0001  -0.0001  0.0000  -0.0000  0.0000  -0.0000
1979  May   -0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  -0.0000  0.0000  -0.0000  0.0000  -0.0000
1979  Jun   -0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  -0.0000  0.0000  -0.0000  0.0000  -0.0000
1979  Jul   -0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  -0.0000  0.0000  -0.0000  0.0000  -0.0000
1979  Aug   -0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  -0.0000  0.0000  -0.0000  0.0000  -0.0000
1979  Sep   -0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  -0.0000  0.0000  -0.0000  0.0000  -0.0000
* -----
*
* -----
* Annual mass balance terms (g) in water layer of water body system of 100.00 m for substance: EXSW2
* (years may be incomplete)
* Year  DelMas  MasIni  MasDrf  MasAtmDep  MasDra  MasRnf  MasSedIn  MasSedOut  MasDwn  MasUps  MasTra  MasFor  MasVol
* -----
1978    0.0000  0.0000  0.1716  0.0000  0.0000  0.8665  -0.0214  0.0202  -18.3659  17.3302  -0.0011  0.0000  -0.0000
1979   -0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0008  -0.0008  0.0000  -0.0000  0.0000  -0.0000
* -----

```

Figure 3.15c The summary output file: mass balance water layer.

```

* Table: Mass balance of substance in the sediment
* Key to the table
* -----
* DelMasSed      Change in mass present in sediment system (g)
* MasIniSed      Mass initially present in sediment (g)
* MasErs         Loading of sediment by erosion (g)
* MasWatIn       Mass transferred to water layer (g)
* MasWatOut      Mass transferred from water layer (g)
* MasDwnSed      Mass flowed across boundary to deeper layers (g)
* MasTraSed      Mass transformed in sediment (g)
* MasFor         Mass formed in sediment (g)
* -----

* -----
* Monthly mass balance terms (g) in sediment of water body system of 100.00 m for substance: EXSW2
* Year  Month  DelMasSed  MasIniSed  MasErs     MasWatIn   MasWatOut   MasDwnSed  MasTra     MasFor
* -----
1978  Oct    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000
1978  Nov    0.0031    0.0000    0.0001    -0.0180   0.0211    0.0000    -0.0000    0.0000    0.0000
1978  Dec   -0.0019    0.0031    0.0000    -0.0022   0.0004    0.0000    -0.0000    0.0000    0.0000
1979  Jan   -0.0003    0.0013    0.0000    -0.0003   0.0000    0.0000    -0.0000    0.0000    0.0000
1979  Feb   -0.0002    0.0009    0.0000    -0.0001   0.0000    0.0000    -0.0000    0.0000    0.0000
1979  Mar   -0.0001    0.0008    0.0000    -0.0001   0.0000    0.0000    -0.0000    0.0000    0.0000
1979  Apr   -0.0001    0.0007    0.0000    -0.0001   0.0000    0.0000    -0.0000    0.0000    0.0000
1979  May   -0.0001    0.0006    0.0000    -0.0000   0.0000    0.0000    -0.0000    0.0000    0.0000
1979  Jun   -0.0001    0.0005    0.0000    -0.0000   0.0000    0.0000    -0.0000    0.0000    0.0000
1979  Jul   -0.0001    0.0005    0.0000    -0.0000   0.0000    0.0000    -0.0000    0.0000    0.0000
1979  Aug   -0.0000    0.0004    0.0000    -0.0000   0.0000    0.0000    -0.0000    0.0000    0.0000
1979  Sep   -0.0000    0.0004    0.0000    -0.0000   0.0000    0.0000    -0.0000    0.0000    0.0000
* -----

* -----
* Annual mass balance terms (g) in sediment of water body system of 100.00 m for substance: EXSW2
* (years may be incomplete)
* Year  DelMasSed  MasIniSed  MasErs     MasWatIn   MasWatOut   MasDwnSed  MasTraSed  MasForSed
* -----
1978    0.0013    0.0000    0.0001    -0.0202    0.0214    0.0000    -0.0001    0.0000
1979   -0.0009    0.0000    0.0000    -0.0008    0.0000    0.0000    -0.0002    0.0000
* -----

```

Figure 3.15d The summary output file: mass balance sediment

```

* -----
* TOXSWA REPORT: Exposure in water body
*
* Table: Annual maximum exposure concentrations in water layer of substance: EXSW2
* In segment from 95.00 to 100.00 m in water body
* -----
* Year                Concentration          Date                Daynr
*                   µg.L-1                      (since start simulation)
* -----
1978                  39.57                25-Nov-1978-02h00    56
1979                  0.000068            01-Jan-1979-07h00    93
*
* Tables: Maximum exposure concentrations in water layer
* In segment from 95.00 to 100.00 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 moment of the period considered
*
* Table: PEC in water layer of substance: EXSW2
* -----
*                   Concentration          Date                Daynr
*                   µg.L-1                      (since start simulation)
* -----
Global max            39.57                25-Nov-1978-02h00    56
(incl. suspend.solids) 39.57                25-Nov-1978-02h00    56)
PECsw_1_day          0.02820              26-Nov-1978-02h00    57
PECsw_2_days         0.007121             27-Nov-1978-02h00    58
PECsw_3_days         0.003477             28-Nov-1978-02h00    59
PECsw_4_days         0.002160             29-Nov-1978-02h00    60
PECsw_7_days         0.000387             02-Dec-1978-02h00    63
PECsw_14_days        1.314                09-Dec-1978-02h00    70
PECsw_21_days        0.01980              16-Dec-1978-02h00    77
PECsw_28_days        0.000048             23-Dec-1978-02h00    84
PECsw_42_days        0.000051             06-Jan-1979-02h00    98
PECsw_50_days        0.000038             14-Jan-1979-02h00   106
PECsw_100_days       0.000010             05-Mar-1979-02h00   156
* -----
* Legend: - in table means PECsw is later than end of simulated period: 30-Sep-1979
*
* Table: Maximum Time Weighted Averaged Exposure Concentrations substance: EXSW2
* -----
*                   Concentration          Date                Daynr
*                   µg.L-1                      (since start simulation)
* -----
TWAEcsw_1_day        16.88                26-Nov-1978-00h00    57
TWAEcsw_2_days       8.448                27-Nov-1978-00h00    58
TWAEcsw_3_days       5.634                28-Nov-1978-00h00    59
TWAEcsw_4_days       4.226                29-Nov-1978-00h00    60
TWAEcsw_7_days       2.415                02-Dec-1978-00h00    63
TWAEcsw_14_days      1.260                28-Nov-1978-09h00    59
TWAEcsw_21_days      0.8402               05-Dec-1978-09h00    66
TWAEcsw_28_days      0.6358               12-Dec-1978-09h00    73
TWAEcsw_42_days      0.4242               26-Dec-1978-09h00    87
TWAEcsw_50_days      0.3569               03-Jan-1979-09h00    95
TWAEcsw_100_days     0.1785               22-Feb-1979-09h00   145
* -----

```

Figure 3.15e The summary output file: exposure concentrations in water.

```

* Tables: Maximum exposure content in sediment
-----
* In the top      5.00 cm sediment located under
* the water body segment from 95.00 to 100.00 m,
* the content is expressed as µg substance per kg dry sediment.

* Table: PEC in sediment of substance: EXSW2
-----
*
*
*          Content          Date          Daynr
*          µg.kg-1          (since start simulation)
* -----
Global max          5.338      25-Nov-1978-11h00      56
PECsed_1_day        1.954      26-Nov-1978-11h00      57
PECsed_2_days       1.420      27-Nov-1978-11h00      58
PECsed_3_days       1.174      28-Nov-1978-11h00      59
PECsed_4_days       1.026      29-Nov-1978-11h00      60
PECsed_7_days       0.7817     02-Dec-1978-11h00      63
PECsed_14_days      0.5864     09-Dec-1978-11h00      70
PECsed_21_days      0.4584     16-Dec-1978-11h00      77
PECsed_28_days      0.3911     23-Dec-1978-11h00      84
PECsed_42_days      0.3135     06-Jan-1979-11h00      98
PECsed_50_days      0.2825     14-Jan-1979-11h00     106
PECsed_100_days     0.1720     05-Mar-1979-11h00     156
* -----
* Legend: - in table means PECsed is later than end of simulated period: 30-Sep-1979

* Table: Maximum Time Weighted Averaged Exposure Content substance: EXSW2
-----
*
*
*          Content          Date          Daynr
*          µg.kg-1          (since start simulation)
* -----
TWAECSed_1_day      3.650      26-Nov-1978-04h00      57
TWAECSed_2_days     2.754      27-Nov-1978-03h00      58
TWAECSed_3_days     2.296      28-Nov-1978-02h00      59
TWAECSed_4_days     2.011      29-Nov-1978-02h00      60
TWAECSed_7_days     1.544      02-Dec-1978-02h00      63
TWAECSed_14_days    1.102      09-Dec-1978-02h00      70
TWAECSed_21_days    0.9058     16-Dec-1978-02h00      77
TWAECSed_28_days    0.7857     23-Dec-1978-02h00      84
TWAECSed_42_days    0.6410     06-Jan-1979-01h00      98
TWAECSed_50_days    0.5863     14-Jan-1979-01h00     106
TWAECSed_100_days   0.4034     05-Mar-1979-01h00     156
* -----

*
* End of TOXSWA REPORT: Exposure in water body
* -----

```

Figure 3.15f The summary output file: exposure concentrations in sediment.

**Exposure concentrations in water**

First a table with the maximum Predicted Environmental Concentrations (PEC) in the last segment downstream in the water body is given for each simulated year. 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.

**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 has the extension `.sum` (`RunId.out`). It gives output selected by the user from the output list in the TOXSWA input file (`.txw`). As described in Section 3.3.13, the output is 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. This type of model output is produced only at the dates specified in the `HorVertProfiles` 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 four types of general format:

(a) for water layer state variables defined at a node:

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

where `n` is determined by the option given by `OptOutputDistances`:

```
All      the number of nodes (distances) in the water layer, or
table    the number of nodes specified in the OutputDistances table, or
None     zero.
```

(b) for water layer fluxes, defined at the interface between two water layer segments:

```
Time      Date      Identifier  Value(0), Value(1)  ....  Value(n)
```

where `n` is the same in in option (a). For all three options, the flux `Value(0)` is given, being the flux at the  $x = 0$ , the upper boundary of the entire waterbody. Note that for the value (`n`) the fluxes are given at the interface of the segments `n` and `n+1`

(c) for sediment state variables defined at a node in the water layer and located in the centre of a sediment layer:

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

where `n` is the node in the water layer, as described for option (a), and where `m` is determined by the option given by `OptOutputDepths`:

```
All      the number of nodes (depths) in the sediment, or
table    the number of nodes specified in the OutputDepths table, or
None     zero.
```

Note that there is no output of fluxes at interfaces of the sediment layers.

(d) Distance and depth independent variables (e.g. mass in the water layer):

```
Time      Date      Identifier  Value
```

---

Figure 3.16 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 found in the 0 - 5 m, 45 - 50 m and 95 - 100 m segments 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 node numbers, distances of the nodal points, and distances of the segment interfaces are listed directly after the header.
4. `OutputDepths` was set at 0.0005 and 0.0085 m. These depths are in the 0 - 0.001 m, and 0.007 - 0.010 m layers with nodal points situated at 0.0005 and 0.085 m distance in the sediment in layer numbers 1 and 14. The distances of the nodal points are listed directly after the header.
5. Output was requested for the variables `QBou`, `DepWat`, `ConLiqWatLay`, `ConSysSed`, `MasWatLay`.
6. The name of the substance is coupled as label to the output variable, when the output variable concerns a substance. In the example `'EXSW2'` in `ConLiqWatLay_EXSW2`.
7. For sediment state variables the node number in the water layer above the selected sediment subsystem is indicated immediately after the output variable (4<sup>th</sup> position in record). In the example `ConSysSed_EXSW2` is shown for layers below water layer segments 1, 10 and 20. At the end of the records where the units are described, we indicated whether the values refer to water layer nodes or the water layer segment interfaces (fluxes) i.e. the following texts are specified: `"(values at segment nodes)"` and `"(values at segment interfaces)"` respectively. For sediment we did not indicate this as all values refer to sediment nodes, because values for fluxes across sediment layer interfaces are not given as output.
8. Only one value is given for `MasWatLay`, because it concerns the total mass in the 20 water layer segments.

```

* -----
* Results from the TOXSWA model (c) Wageningen University & Research
* FOCUS TOXSWA version : 5.5.3
* TOXSWA model version : 3.3.6
* TOXSWA created on : 17-Dec-2017

* Working directory : C:\SwashProjects\Project_1\TOXSWA
* Run ID : 3
* Input file generated on : 25-09-2018
* -----

Depths of sediment nodes for output in Z-direction: 0.500000E-03 0.850000E-01
Distances of water layer nodes for output in X-direction: 0.250000E+01 0.475000E+02 0.975000E+02
Distances of water layer segment interfaces for output in X-direction: 0.000000E+00 0.500000E+01 0.500000E+02 0.100000E+03
* Option PrintCumulatives was set to false
* Option OptCalcStabilitySediment was set to true
* Option OptCalcStabilityWater was set to true
* Unit for QBou is (m3.s-1) (values at segment interfaces)
0.000 01-Oct-1978-00h00 QBou 0.255700E-02 0.255700E-02 0.255900E-02 0.256000E-02
* Unit for ConLiqWatLay is (g.m-3) (values at segment nodes)
0.000 01-Oct-1978-00h00 ConLiqWatLay_EXSW2 0.000000E+00 0.000000E+00 0.000000E+00
* Unit for ConSysSed is (g.m-3)
0.000 01-Oct-1978-00h00 ConSysSed_EXSW2 1 0.000000E+00 0.000000E+00
0.000 01-Oct-1978-00h00 ConSysSed_EXSW2 10 0.000000E+00 0.000000E+00
0.000 01-Oct-1978-00h00 ConSysSed_EXSW2 20 0.000000E+00 0.000000E+00
* Unit for MasWatLay is (g)
0.000 01-Oct-1978-00h00 MasWatLay_EXSW2 0.000000E+00
.

```

Figure 3.16 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 are produced only at times specified in the `HorVertProfiles` table. For each requested point in time and for each substance, a series of records is produced with the name `XProfile_subst` and `ZProfile_subst` (where `subst` must be substituted by the appropriate substance name). The records in the output give the following variables:

Horizontal profile for the water layer

- Day number from start of simulation
- Date and time
- Xprofile label indicating horizontal profile in water layer and substance name
- Distance middle of segment (= grid point) from start of water body (m)
- Water depth (m)
- Total concentration in water ( $\text{g m}^{-3}$ )
- Dissolved concentration in water ( $\text{g m}^{-3}$ )

Vertical profile for the sediment

- Day number from start of simulation
- Date and time
- Zprofile label indicating vertical profile in sediment and substance name
- Segment number in water layer, below which vertical profile in sediment is given
- Depth middle of sediment layer (= grid point) (m)
- Pore fraction, ( $\text{m}^3 \text{m}^{-3}$ )
- Total concentration in the sediment ( $\text{g m}^{-3}$ )
- Dissolved concentration in the sediment ( $\text{g m}^{-3}$ )

Values for water that are given in the out file are for all water layer segments. Values for sediment are given for all sediment layers below water layer segments selected via `OptOutputDistances`. See Sections 3.3.13 and 3.7.1. for more details on this selection. In the example output is given for all sediment layers 1 to 14, under water layer segment 1, 10 and 20 (see Figure 3.17)

```

60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.250000E+01 0.411760E+00 0.125667E-06 0.125657E-06
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.750000E+01 0.411760E+00 0.191298E-06 0.191283E-06
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.125000E+02 0.411760E+00 0.258371E-06 0.258351E-06
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.175000E+02 0.411760E+00 0.326948E-06 0.326922E-06
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.225000E+02 0.411760E+00 0.397085E-06 0.397053E-06
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.275000E+02 0.411760E+00 0.468827E-06 0.468790E-06
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.325000E+02 0.411760E+00 0.542217E-06 0.542175E-06
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.375000E+02 0.411760E+00 0.617291E-06 0.617242E-06
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.425000E+02 0.411760E+00 0.694094E-06 0.694040E-06
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.475000E+02 0.411760E+00 0.772641E-06 0.772581E-06
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.525000E+02 0.411760E+00 0.852938E-06 0.852871E-06
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.575000E+02 0.411760E+00 0.934964E-06 0.934891E-06
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.625000E+02 0.411760E+00 0.101864E-05 0.101857E-05
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.675000E+02 0.411760E+00 0.110384E-05 0.110375E-05
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.725000E+02 0.411760E+00 0.119016E-05 0.119007E-05
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.775000E+02 0.411760E+00 0.127687E-05 0.127677E-05
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.825000E+02 0.411760E+00 0.136242E-05 0.136231E-05
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.875000E+02 0.411760E+00 0.144371E-05 0.144360E-05
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.925000E+02 0.411760E+00 0.151458E-05 0.151447E-05
60.000 30-Nov-1978-00h00 XProfile_EXSW2 0.975000E+02 0.411760E+00 0.156253E-05 0.156240E-05
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.500000E-03 0.600000E+00 0.436238E-03 0.913396E-04
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.150000E-02 0.600000E+00 0.126352E-02 0.264555E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.250000E-02 0.600000E+00 0.197279E-02 0.413063E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.350000E-02 0.600000E+00 0.250871E-02 0.525274E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.500000E-02 0.600000E+00 0.300825E-02 0.629868E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.700000E-02 0.600000E+00 0.284959E-02 0.596648E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.900000E-02 0.600000E+00 0.219425E-02 0.459432E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.125000E-01 0.600000E+00 0.807263E-03 0.169025E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.175000E-01 0.600000E+00 0.152233E-03 0.318745E-04
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.250000E-01 0.600000E+00 0.843166E-05 0.176542E-05
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.350000E-01 0.600000E+00 0.339708E-06 0.711281E-07
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.450000E-01 0.600000E+00 0.174423E-07 0.365208E-08
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.600000E-01 0.600000E+00 0.388613E-09 0.813680E-10
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 1 -0.850000E-01 0.600000E+00 0.347829E-11 0.728286E-12
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.500000E-03 0.600000E+00 0.524500E-03 0.109820E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.150000E-02 0.600000E+00 0.151278E-02 0.316746E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.250000E-02 0.600000E+00 0.235853E-02 0.493830E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.350000E-02 0.600000E+00 0.299538E-02 0.627173E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.500000E-02 0.600000E+00 0.358490E-02 0.750607E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.700000E-02 0.600000E+00 0.338505E-02 0.708762E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.900000E-02 0.600000E+00 0.260007E-02 0.544403E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.125000E-01 0.600000E+00 0.956793E-03 0.200334E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.175000E-01 0.600000E+00 0.188258E-03 0.394176E-04
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.250000E-01 0.600000E+00 0.133225E-04 0.278947E-05
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.350000E-01 0.600000E+00 0.895757E-06 0.187554E-06
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.450000E-01 0.600000E+00 0.725290E-07 0.151861E-07
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.600000E-01 0.600000E+00 0.197952E-08 0.414472E-09
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 10 -0.850000E-01 0.600000E+00 0.187589E-10 0.392775E-11
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.500000E-03 0.600000E+00 0.631292E-03 0.132180E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.150000E-02 0.600000E+00 0.181416E-02 0.379850E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.250000E-02 0.600000E+00 0.282449E-02 0.591393E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.350000E-02 0.600000E+00 0.358246E-02 0.750097E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.500000E-02 0.600000E+00 0.427878E-02 0.895892E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.700000E-02 0.600000E+00 0.402592E-02 0.842947E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.900000E-02 0.600000E+00 0.308252E-02 0.645418E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.125000E-01 0.600000E+00 0.113019E-02 0.236639E-03
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.175000E-01 0.600000E+00 0.228022E-03 0.477434E-04
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.250000E-01 0.600000E+00 0.183520E-04 0.384254E-05
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.350000E-01 0.600000E+00 0.144980E-05 0.303560E-06
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.450000E-01 0.600000E+00 0.126748E-06 0.265386E-07
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.600000E-01 0.600000E+00 0.353298E-08 0.739736E-09
60.000 30-Nov-1978-00h00 ZProfile_EXSW2 20 -0.850000E-01 0.600000E+00 0.335794E-10 0.703086E-11

```

Figure 3.17 The comprehensive output file; an excerpt of the profile output (date for which profiles are requested is 30 November 1978).

### 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 (Name.meteo) and subsequently translated to temperatures for each hour in the runID.meteo file. The intermediate output files runID.hyd and runID.meteo 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 3.18. 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. Hence, the water depth is constant over the entire length of the water body for the FOCUS Surface Water scenarios, a single value for the water depth is given at the end of the record.

```

* Time Date Qbou (0) QBou (1) DepWat
* (m3.s-1) (m3.s-1) (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 3.18 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 3.19. 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 3.19 The intermediate output file runID.tem



# 4 User's guide for the FOCUS\_TOXSWA user interface

## 4.1 Introduction

This chapter gives an overview of the FOCUS\_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).

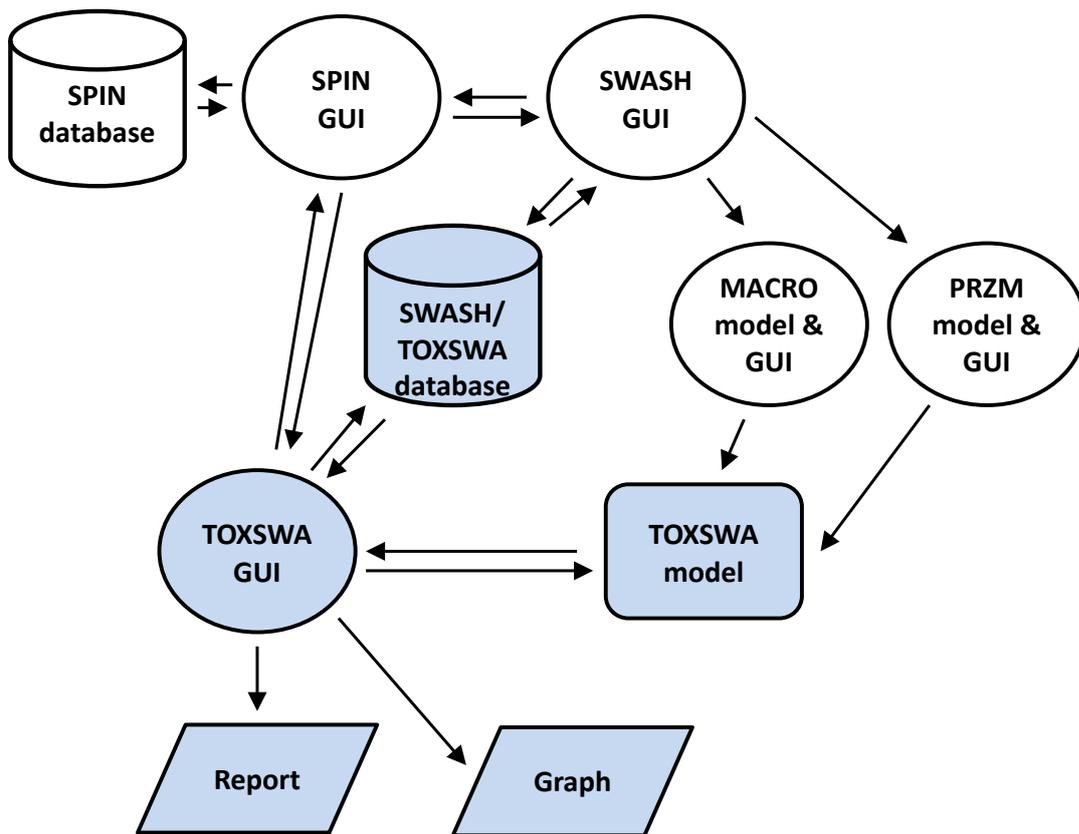


Figure 4.1 Overview of the FOCUS\_TOXSWA modelling system (in blue) and its relations with SWASH, SPIN, and the MACRO and PRZM models.

The FOCUS\_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 Section 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 FOCUS\_TOXSWA Graphical User Interface, you do not need to bother about all the relationships. The FOCUS\_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.

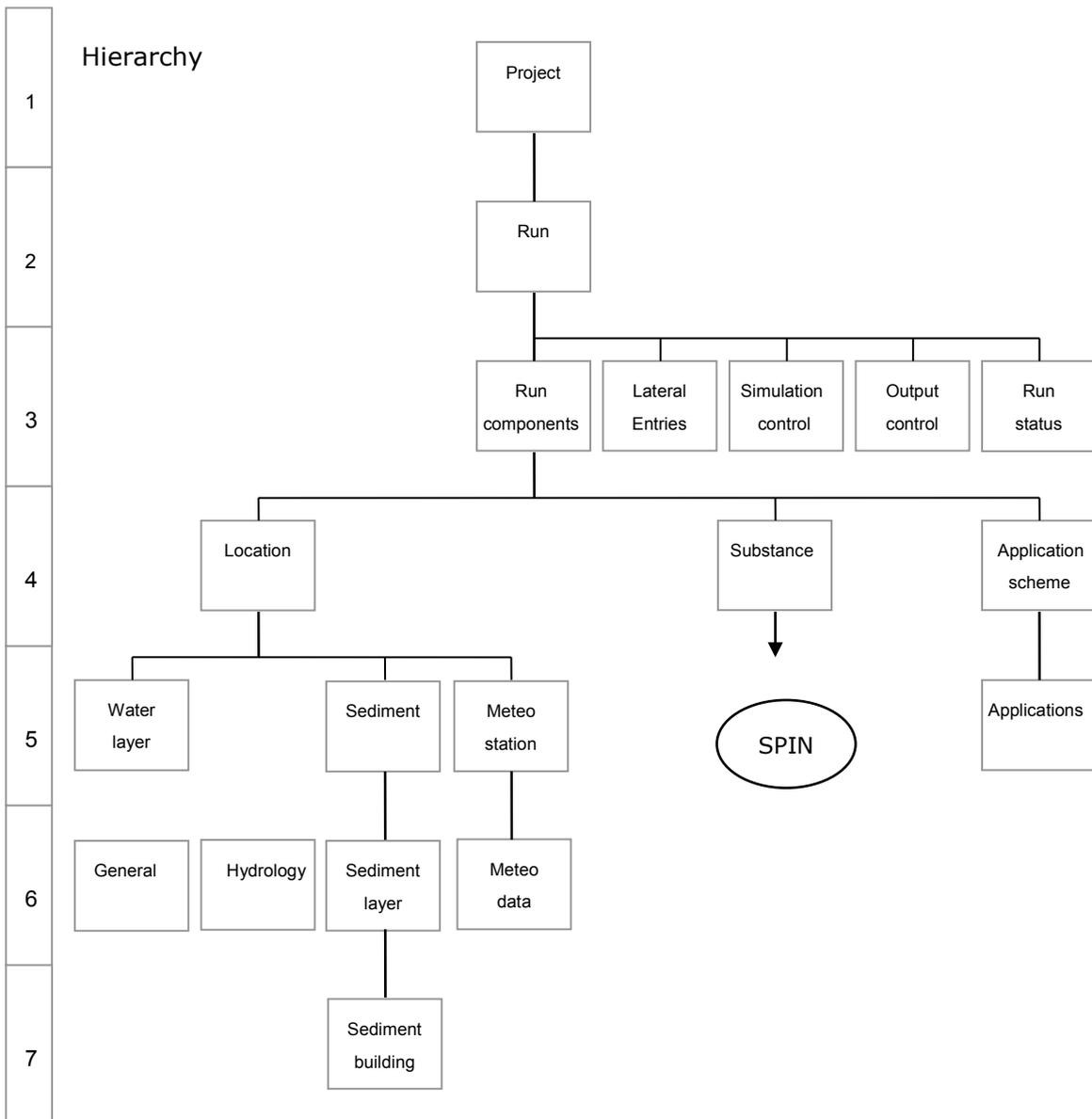


Figure 4.2 Hierarchies within the TOXSWA GUI.

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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 is subdivided into sediment layers (level 6). The sediment 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 (when the option shortcut to desktop was selected 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 Forum for the Co-ordination of pesticide fate models and their Use, FOCUS. Generating FOCUS projects and runs can only be done in SWASH (Van den Berg *et al.*, 2015). SWASH only prepares standard Step 3 FOCUS runs. These can be executed via the TOXSWA GUI. The substance 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

### 4.4.1 General

FOCUS runs are organized in so-called projects: specific combinations of a substance, a crop and an application scheme. Consequently, 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 (Van den Berg *et al.*, 2015) 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:

#### Start SWASH

Define the substance or select an already defined substance from the SPIN database (connection automatically from SWASH)

Use the FOCUS wizard to define a project for the specified substance and crops you wish to consider 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

Press the button 'Export FOCUS input to MACRO, PRZM and TOXSWA' with all options selected.

Print the project report.

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.

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

Exit the MACRO shell and enter SWASH again

Click on the PRZM button on the upper bar of the SWASH main window to start the PRZM shell and SWASH closes

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

Exit the PRZM shell and enter SWASH again

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'

Click on the TOXSWA button on the upper bar of the SWASH window to start the TOXSWA shell, and the SWASH shell closes

You will now enter the 'TOXSWA – Projects' window from where you can proceed.

#### 4.4.2 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 execution of 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 (input file), 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 4.11 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, the water layer segment lengths and sediment layer thickness 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 modify the numerical discretization (i.e. shorten the segment lengths/reduce the thickness of the sediment layers) and/or shorten time steps (see also Section 4.4.4).

#### 4.4.3 Viewing the results

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

4. An overview of the applications and pesticide entries of the two entry routes: spray drift and drainage or runoff/erosion.
5. The Global Maximum Concentration in water and in sediment
6. 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.

#### 4.4.4 Special cases: substances with $K_{oc}$ higher than 30,000 L/kg

The TOXSWA GUI selects the standard FOCUS layering with 14 layers 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 30,000 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 30,000 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 layers in the sediment. Therefore, the GUI selects the FOCUS\_highKoc sediment layering with 23 layers for FOCUS Step 3 runs with substances with  $K_{oc}$  values above 30000 L/kg. 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 layering is not selected automatically. The user can change the sediment layering. 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 layering.

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

FOCUS\_TOXSWA 5.5.3 simulates the formation of metabolites in water and in sediment. A consequence 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 primary 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 TOXSWA\_GUI the correction factors  $CF_{m,up}$  can be viewed (FOCUS Step 3 calculations) or entered or changed (FOCUS Step 4 calculations) at the Edit runs form accessed via the Entries tab, in the section Upstream catchment entries (Figure 4.3a). By clicking the button CF the CF form can be accessed (Figure 4.3b).

The screenshot shows the 'Edit Run' dialog box with the 'Entries' tab selected. The 'Upstream catchment entries' section includes a 'CF' button. Other fields include 'Type: Runoff', 'File name: C:\\$washProjects\CProject\_2\PRZM\cereals\_winter\00092-C1.p2', 'Model: PRZM', 'Loading fluxes: Hourly', 'Thickness sediment layer, to which mass sorbed to eroded soil is added (m): 0.01', 'Runoff: Fraction infiltrating, draining to waterbody (0-1): 0.03', 'Start position (m): 0', and 'End position (m): 100'.

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

The screenshot shows the 'Browse Correction Factor for formation of primary water metabolites' dialog box. It contains a table with the following data:

SubstanceCode	Correction Factor
METW1	0.013

Below the table, there is an 'Edit Correction Factor for formation of primary water metabolite' section with fields for 'SubstanceCode water metabolite: METW1' and 'Correction factor metabolite formation in upstream catchment (0 - 1): 0.013'. Buttons for 'Close', 'Cancel', and 'Help' are at the bottom.

Figure 4.3b Browse Correction Factor water metabolites form.

The correction factor needs to be calculated by the user according to the description given in Annex 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. 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.

## 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.

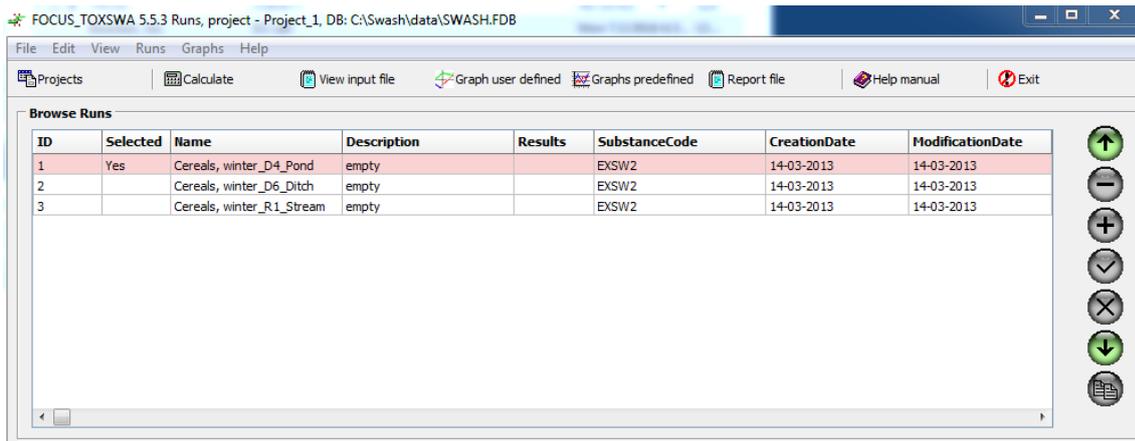


Figure 4.4 The browse box of the Runs form

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.

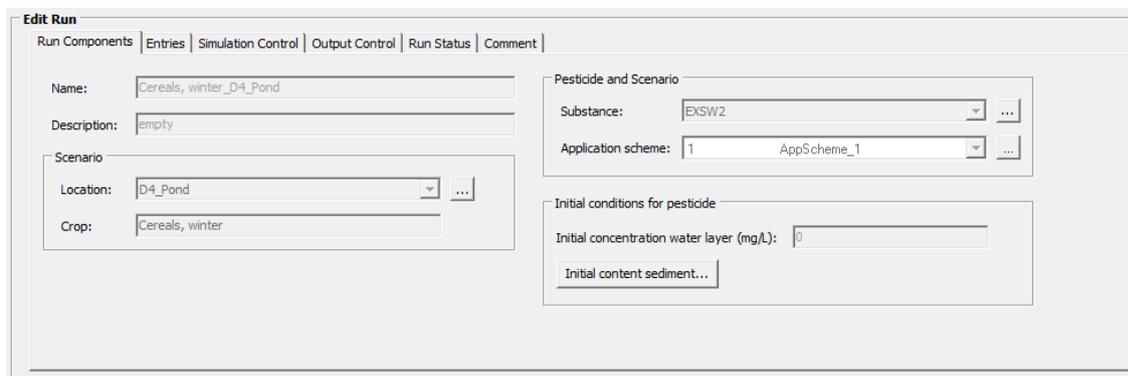
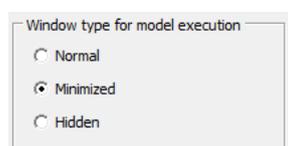


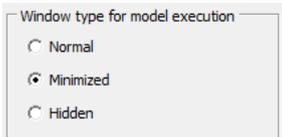
Figure 4.5 The edit box of the Runs form

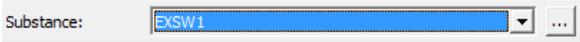
In the edit box of a form the user can edit the record selected in the browse box.

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.

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.

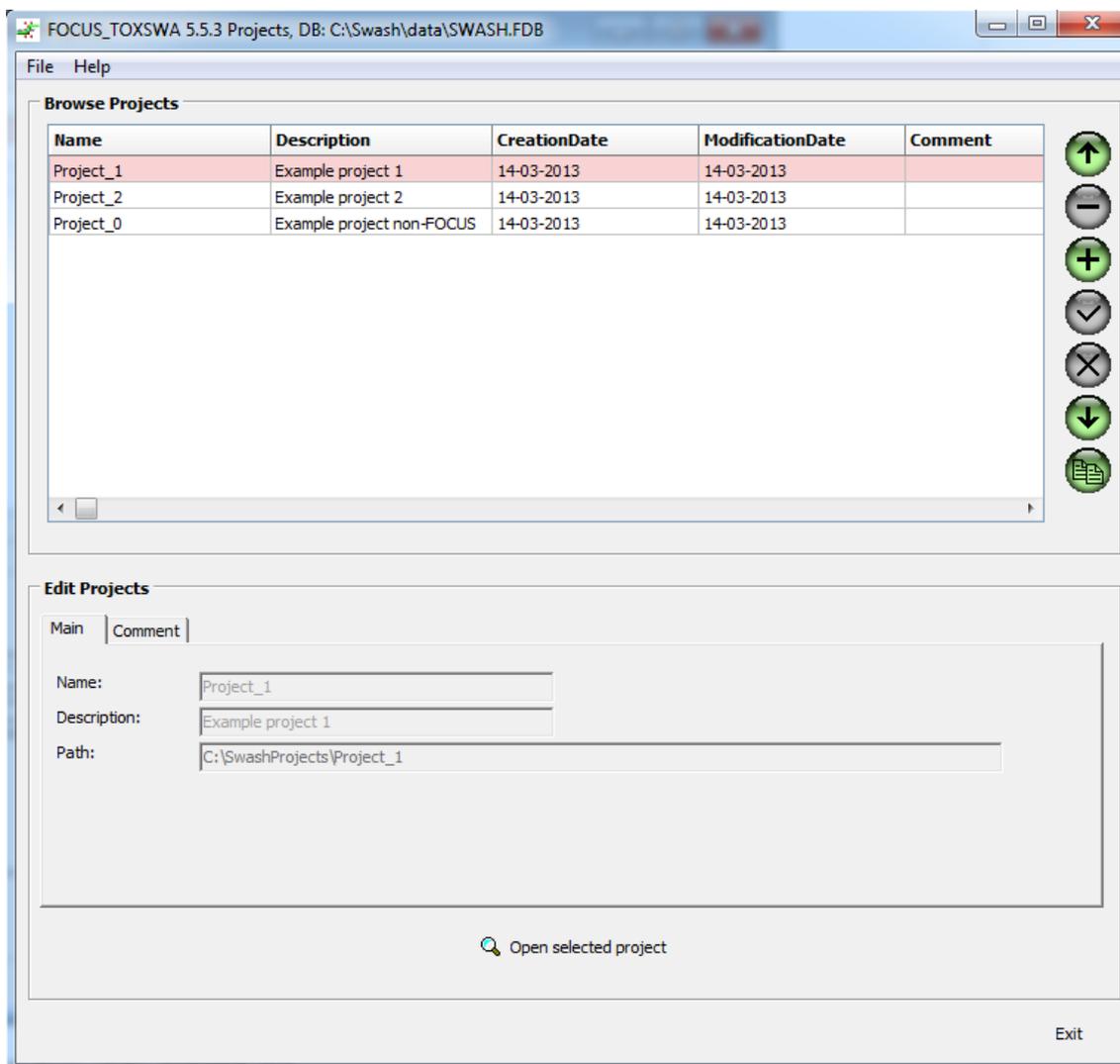


Figure 4.6 The Projects form of the TOXSWA GUI

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

### 4.7.1 General

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).

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 4.7.5 to 4.7.10.

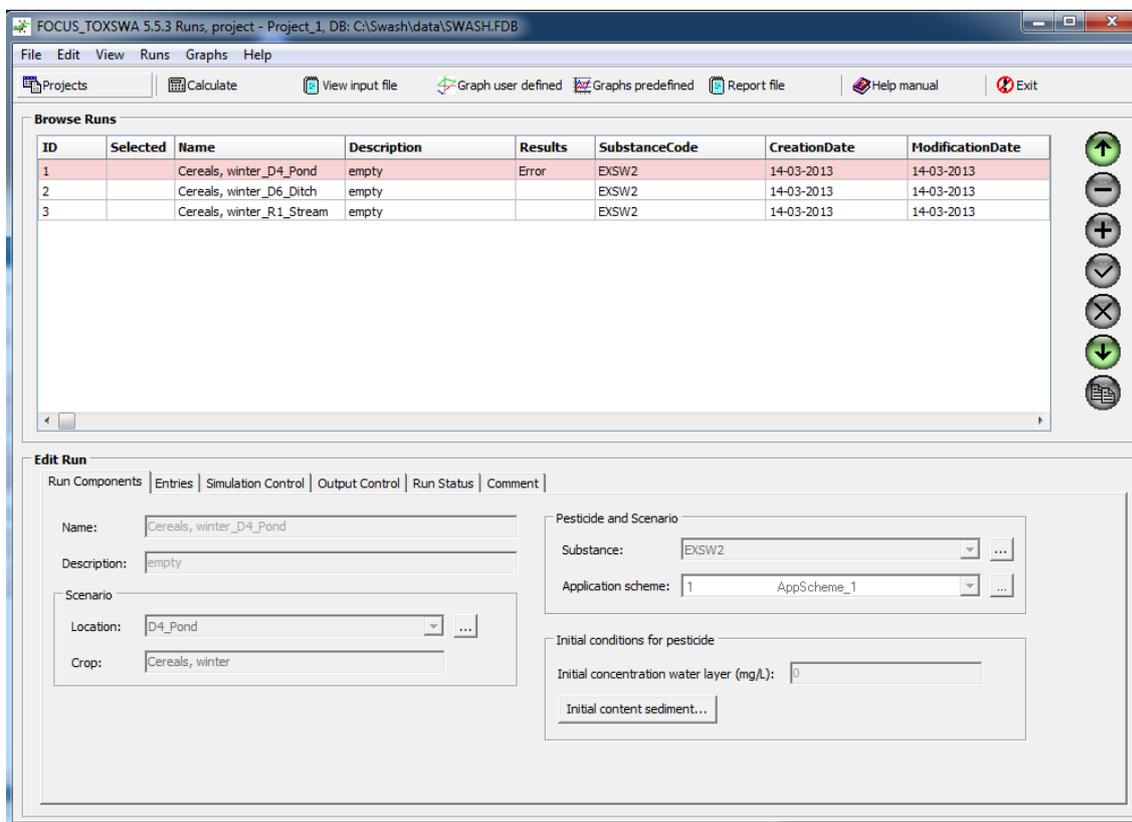


Figure 4.7 The Runs form of the TOXSWA GUI

#### 4.7.2 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)

Option	Sub option	Action
	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
	Addendum manual for version 5.5.3	Opens addendum to manual of version 4.4.2 <sup>7</sup>
	TOXSWA website	Opens TOXSWA's homepage on <a href="http://www.PesticideModels.eu">http://www.PesticideModels.eu</a>
	Whats new	Opens a document describing the new added features
	About	Shows details on development

### 4.7.3 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.

### 4.7.4 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

<sup>7</sup> Note that this field is redundant when this manual has replaced the manual of version 4.4.2 via "Help manual".

---

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.

#### 4.7.5 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.

The screenshot shows the 'Edit Run' dialog box with the 'Run Components' tab selected. The form is organized into several sections:

- Name:** Cereals, winter\_D4\_Pond
- Description:** empty
- Scenario:**
  - Location:** D4\_Pond
  - Crop:** Cereals, winter
- Pesticide and Scenario:**
  - Substance:** EXSW2
  - Application scheme:** 1 (AppScheme\_1)
- Initial conditions for pesticide:**
  - Initial concentration water layer (mg/L):** 0
  - Initial content sediment...** (button)

Figure 4.8 Run Components tab of the Runs form

### Scenario

The 'Location' field gives access to the water layer (including hydrology), sediment, 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.

## 4.7.6 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 list 'Type'. The file name, including its path (table Soil substance files<sup>8</sup>), 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 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

<sup>8</sup> Names in *courier* letter type refer to the name of the variable in the TOXSWA input file

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 correction factors  $CF_{m,up}$  can be viewed (FOCUS Step 3 calculations) or entered or changed (FOCUS Step 4 calculations) by clicking the button CF the CF form can be accessed (see Figure 4.3b). For a further explanation see Section 4.4.

Figure 4.9 Entries tab of the Runs form; runoff calculated with the PRZM model

### 4.7.7 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).

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).

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 3.3.5 of this report.

The following options can be selected:

- OffLine:** TOXSWA assumes that the module has already been run. The program uses an existing file that was generated in a previous run: a hydrological data file (*RunId.hyd*) and/or a temperature data file (*RunId.tem*).
- OnLine:** TOXSWA generates the data files.
- Automatic:** TOXSWA checks if the data file is already available. If so, the hydrological/temperature calculations will be skipped.
- Only:** The hydrological/temperature module is run, but the remainder of the simulations (i.e. concentrations and mass balances of the substance(s) in the water body) is skipped.

## 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 (*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*). The latter is not possible in this version of the GUI.

### 4.7.8 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 Section 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.

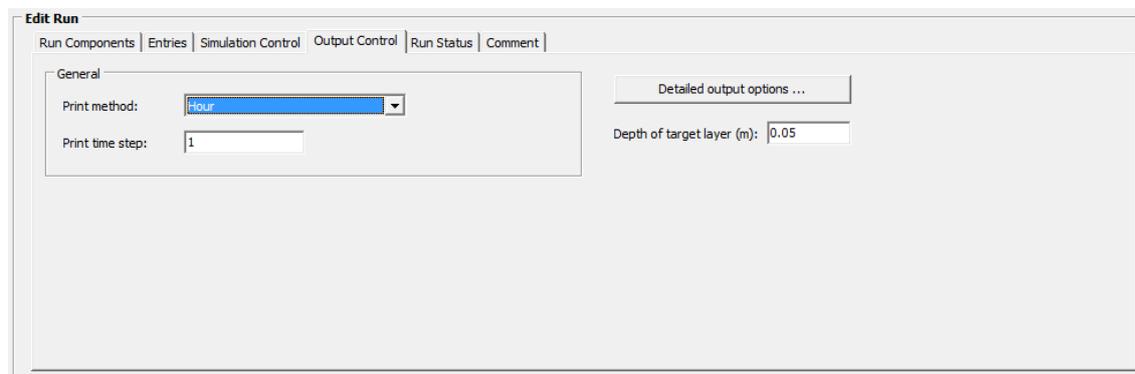


Figure 4.11 Output Control tab of the Runs form

## 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. 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

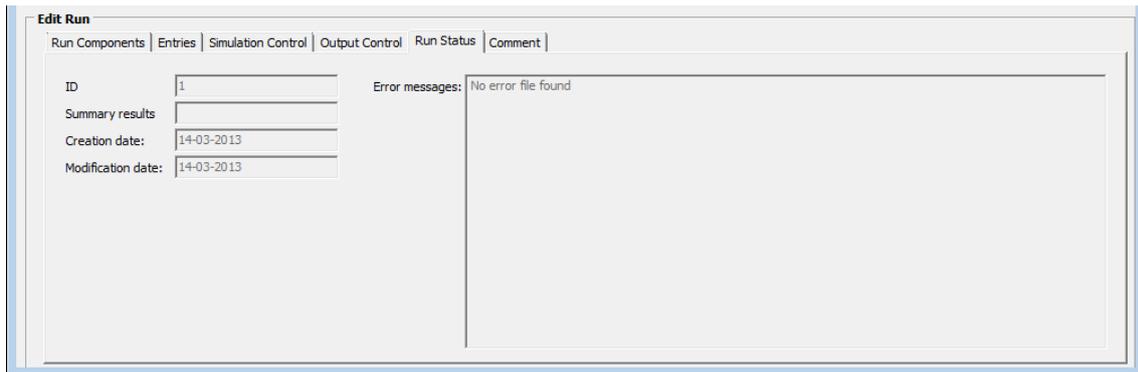
---

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.

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

#### 4.7.9 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).



Edit Run					
Run Components	Entries	Simulation Control	Output Control	Run Status	Comment
ID	1	Error messages: No error file found			
Summary results					
Creation date:	14-03-2013				
Modification date:	14-03-2013				

Figure 4.12 Run Status tab of the Runs form

#### 4.7.10 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

### 4.8.1 General

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 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 4.8.4).

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 5.5.3, the seepage options are not used.

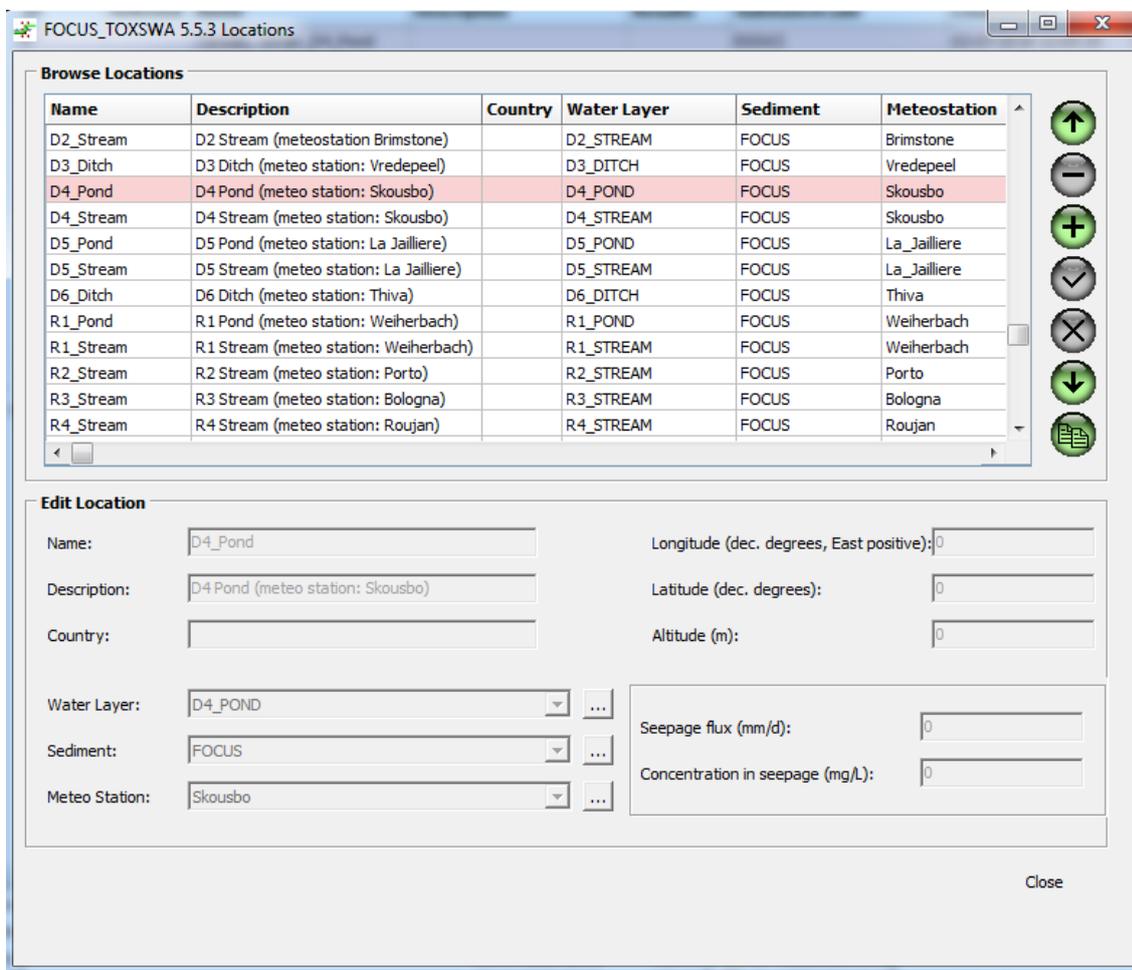


Figure 4.13 The Locations form

#### 4.8.2 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 m<sup>2</sup> bottom area (`AmaMphWatLay`).

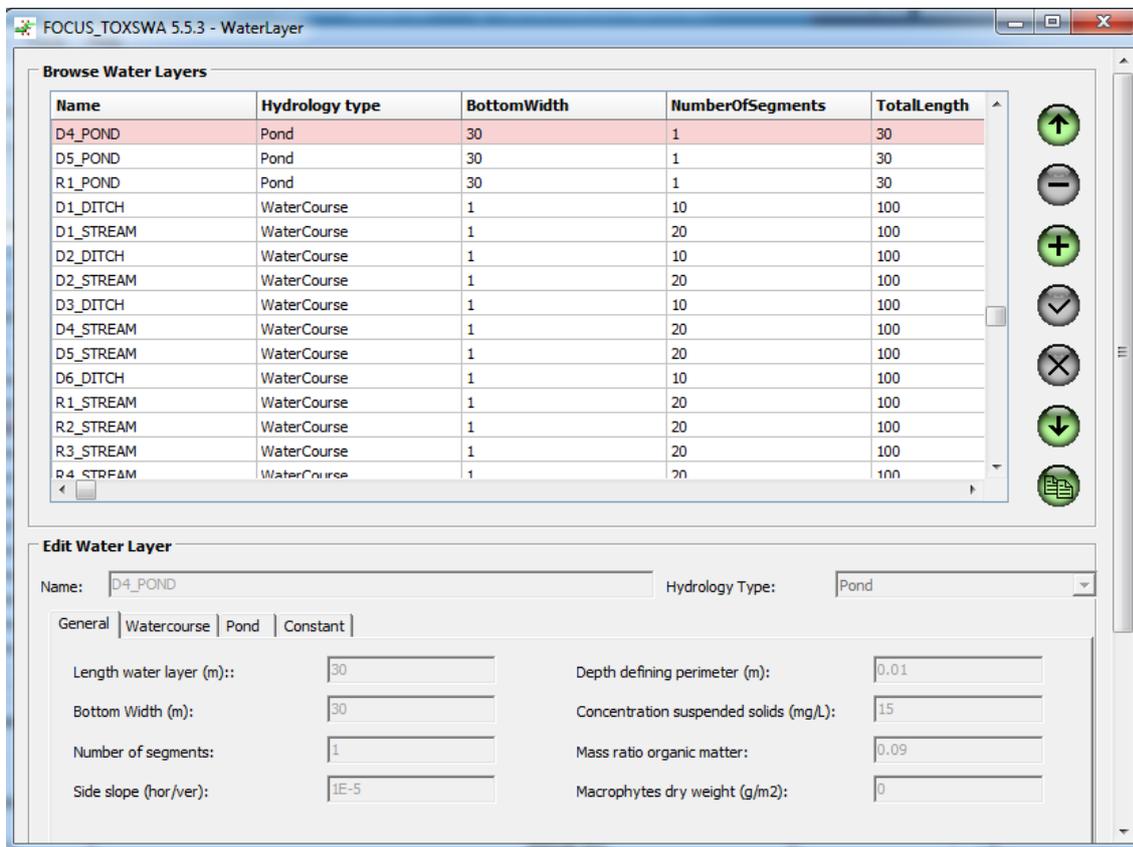


Figure 4.14 The Water layers form, with the General tab opened on the bottom half.

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. mesocosms 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' ( $QB_{asWatCrsInp}$ ), the 'Upstream area' ( $Area_{UpsWatCrsInp}$ ) delivering its water (and sometimes pesticide fluxes) into the watercourse, the 'Width plot along watercourse' ( $WidFldDra$  for drainage,  $WidFldRnf$  for runoff) contributing drainage or runoff fluxes (water and pesticide) and 'Margin erosion' ( $WidFldErs$ ) contributing pesticide sorbed onto eroded soil fluxes to the watercourse.

The dispersion coefficient option ( $OptDis$ ) 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 (see Annex 7). If the option is constant, the value of the 'Dispersion coefficient' ( $CofDisPhsInp$ ) 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' ( $LenRepCha$ ), 'Bottom slope' ( $SloBotRepCha$ ), 'Bottom width' of the channel ( $WidBotRepCha$ ), 'Side slope' ( $SloSidRepCha$ ), constant 'Base flow' ( $QBasRepCha$ ), the 'Upstream area' of the catchment ( $AreaUpStrRepCha$ ), 'Weir height' of the weir crest above the channel bottom of the channel ( $HgtCreRepCha$ ), 'Weir width' i.e. crest width of the weir located at the outflow of the channel ( $WidCreRepCha$ ), 'K-Manning'; bottom roughness at 1 m water depth ( $CofRghRef$ ) and 'Alpha', the energy coefficient, resulting from the non-uniform distribution of flow velocities over a channel cross section ( $CofVelHea$ ).

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.

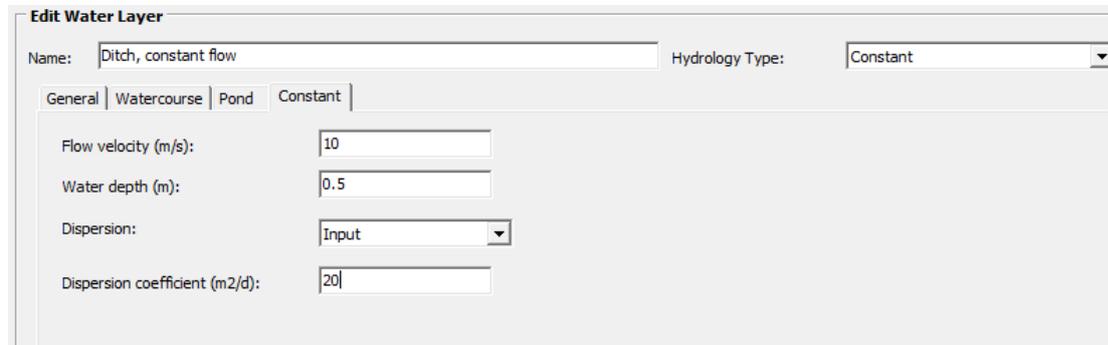
Figure 4.16 The Ponds tab of the Water layers form.

In this form values can be entered for the 'Contributing area' of the pond ( $AeraSurPndInp$ ), the 'Base flow' into the pond ( $QBasePndInp$ ), the 'Height' and 'Width' of the weir ( $HgtCrePnd$ ,  $WidCrePnd$ ) controlling the outflow of the pond and the area from which erosion, 'Area erosion', may enter the pond ( $AreaErsSurPndInp$ ). 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.

## 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.



The screenshot shows the 'Edit Water Layer' dialog box with the 'Constant' tab selected. The 'Name' field contains 'Ditch, constant flow' and the 'Hydrology Type' dropdown is set to 'Constant'. The 'Constant' tab is active, showing the following fields:

Flow velocity (m/s):	10
Water depth (m):	0.5
Dispersion:	Input
Dispersion coefficient (m2/d):	20

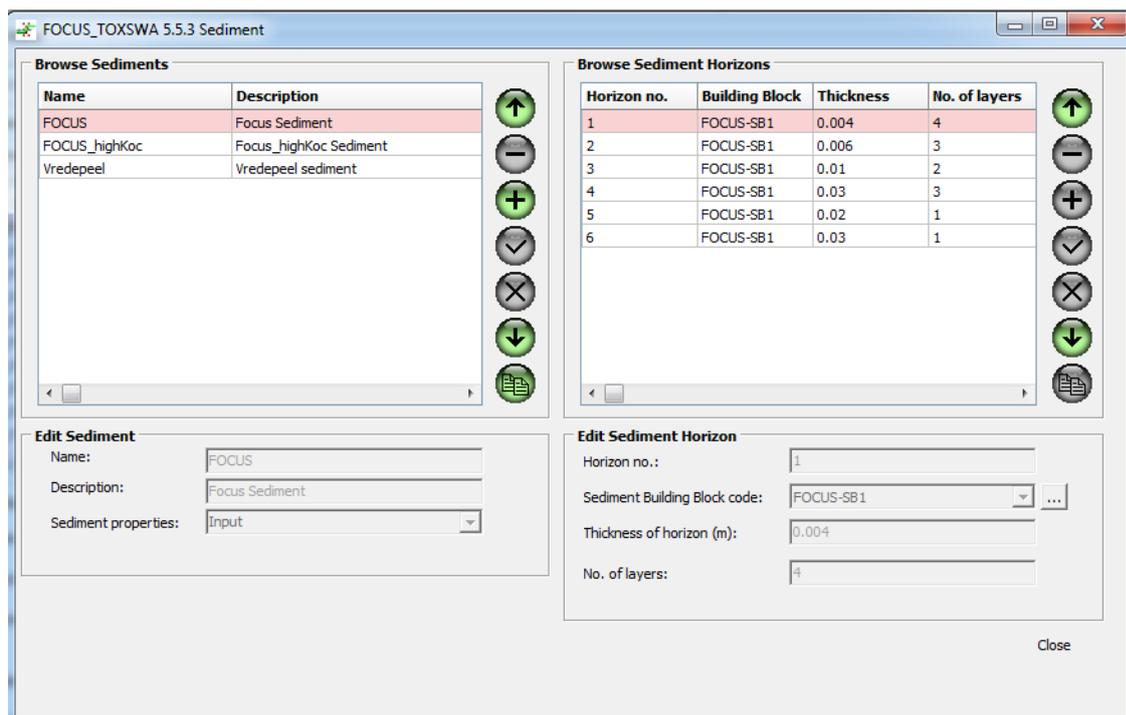
Figure 4.17 The Constant tab of the Water layers form.

## 4.8.3 The Sediment form

The Sediment form can be accessed by pressing the  button behind the pick list of the option field 'Sediment' 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 horizons. In the right half (Browse sediment horizons) properties of individual sediment horizon 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 3.3.8). For more details about the estimation of sediment properties see also Annex 6.



The screenshot shows the 'FOCUS\_TOXSWA 5.5.3 Sediment' dialog box. It is divided into four main sections:

- Browse Sediments:** A table with columns 'Name' and 'Description'. It lists 'FOCUS', 'FOCUS\_highKoc', and 'Vredepeel'.
- Browse Sediment Horizons:** A table with columns 'Horizon no.', 'Building Block', 'Thickness', and 'No. of layers'. It lists 6 horizons for 'FOCUS-SB1'.
- Edit Sediment:** Fields for 'Name' (FOCUS), 'Description' (Focus Sediment), and 'Sediment properties' (Input).
- Edit Sediment Horizon:** Fields for 'Horizon no.' (1), 'Sediment Building Block code' (FOCUS-SB1), 'Thickness of horizon (m)' (0.004), and 'No. of layers' (4).

Figure 4.18 The Sediments form

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 horizons section on the right side of the Sediment form the horizons of the sediment are defined. The sediment consists of a number of horizons, which on their turn are composed of layers. The properties of each horizon are defined by the selected Building Block. In the Edit sediment horizon section the user can modify the different layers by specifying the 'Sub layer no.' ( $N_r$ ), the 'Sediment Building block code', the 'Thickness' ( $Thi_{Hor}$ ) of the layer and the 'Number of layers' ( $Num_{Lay}$ ) in the layer. A new sediment layer can be added with the + button of the navigator or an existing sediment horizon can be copied.

### 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 field<sup>9</sup>.

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.

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 Building Block**

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

<sup>9</sup> 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.

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

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

#### 4.8.4 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.

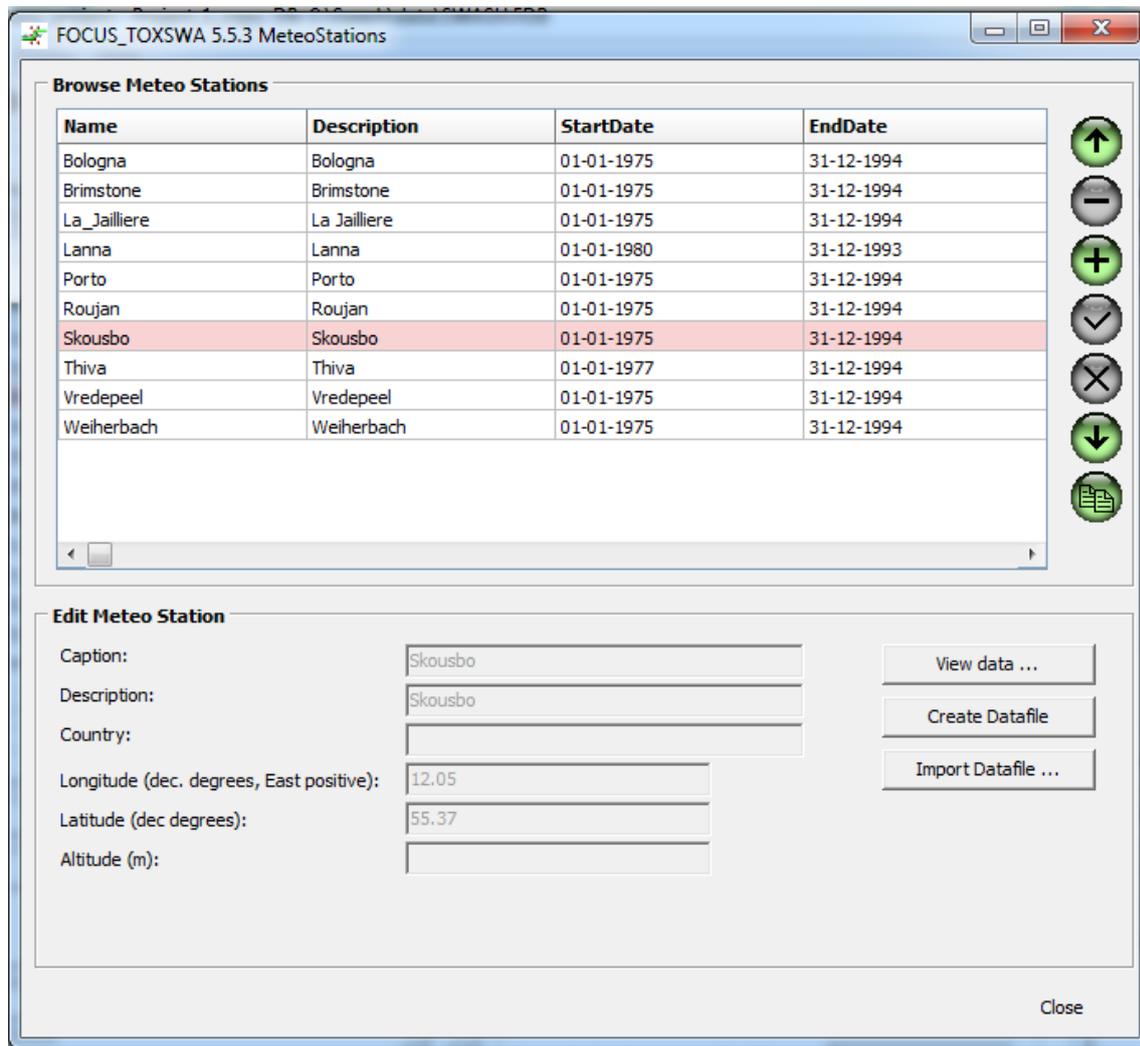


Figure 4.20 The Meteo Stations form

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 4.8.1).

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.

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.

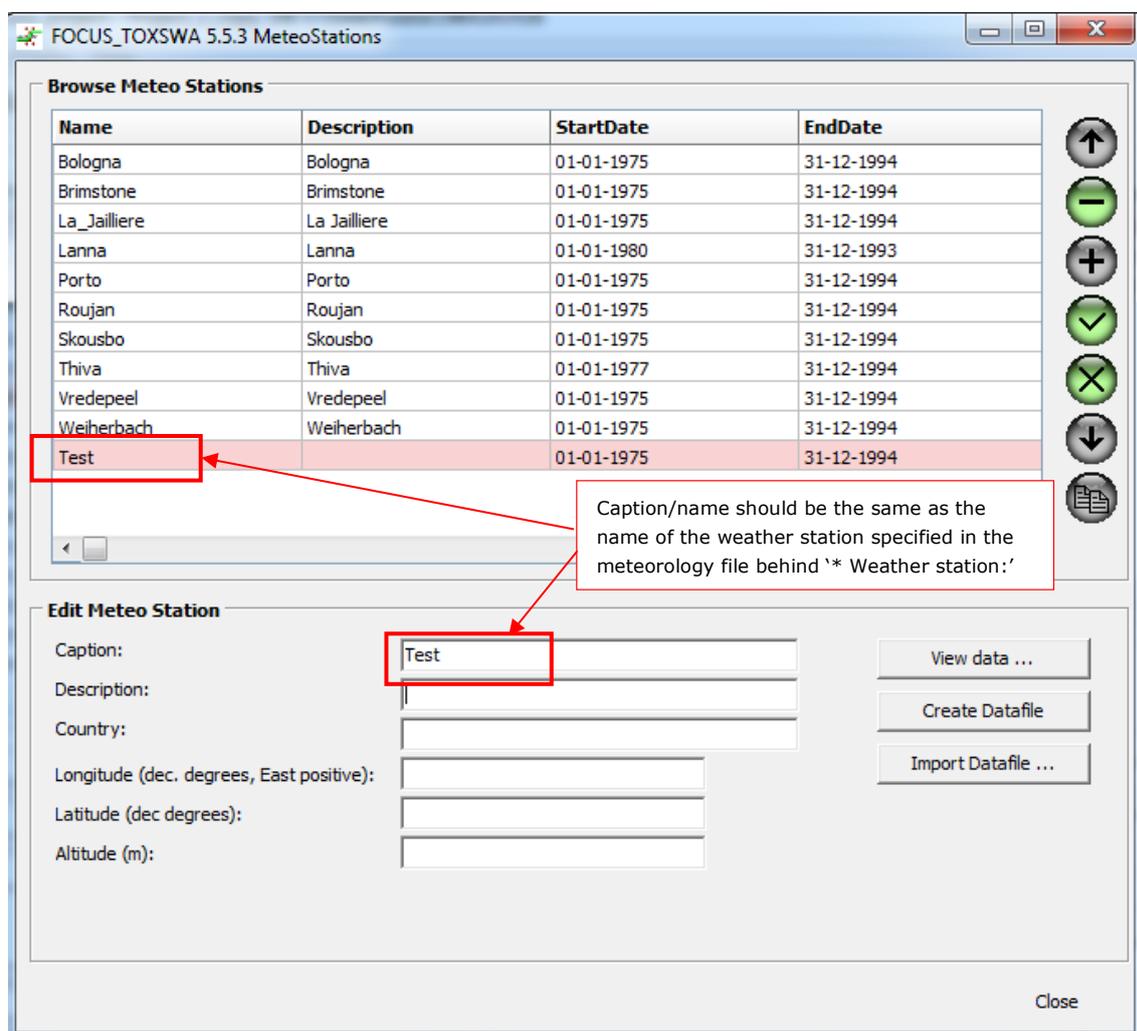


Figure 4.21 The meteo stations form for the example water-sediment study

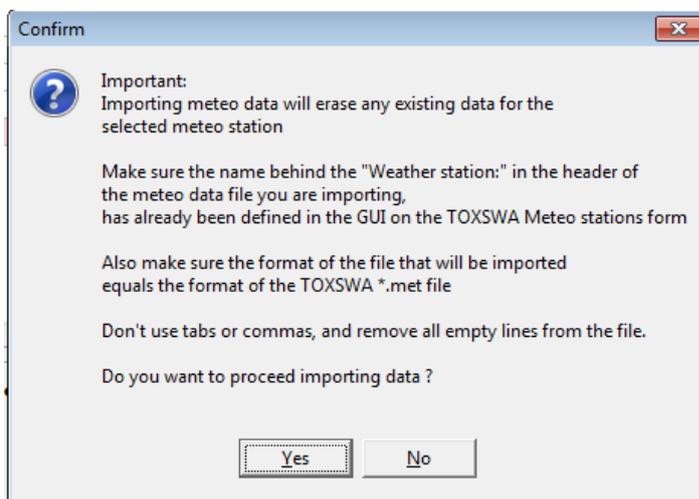


Figure 4.22 Window with instructions shown after pressing the button 'Import Datafile ...' in the Meteo Stations form

## 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.

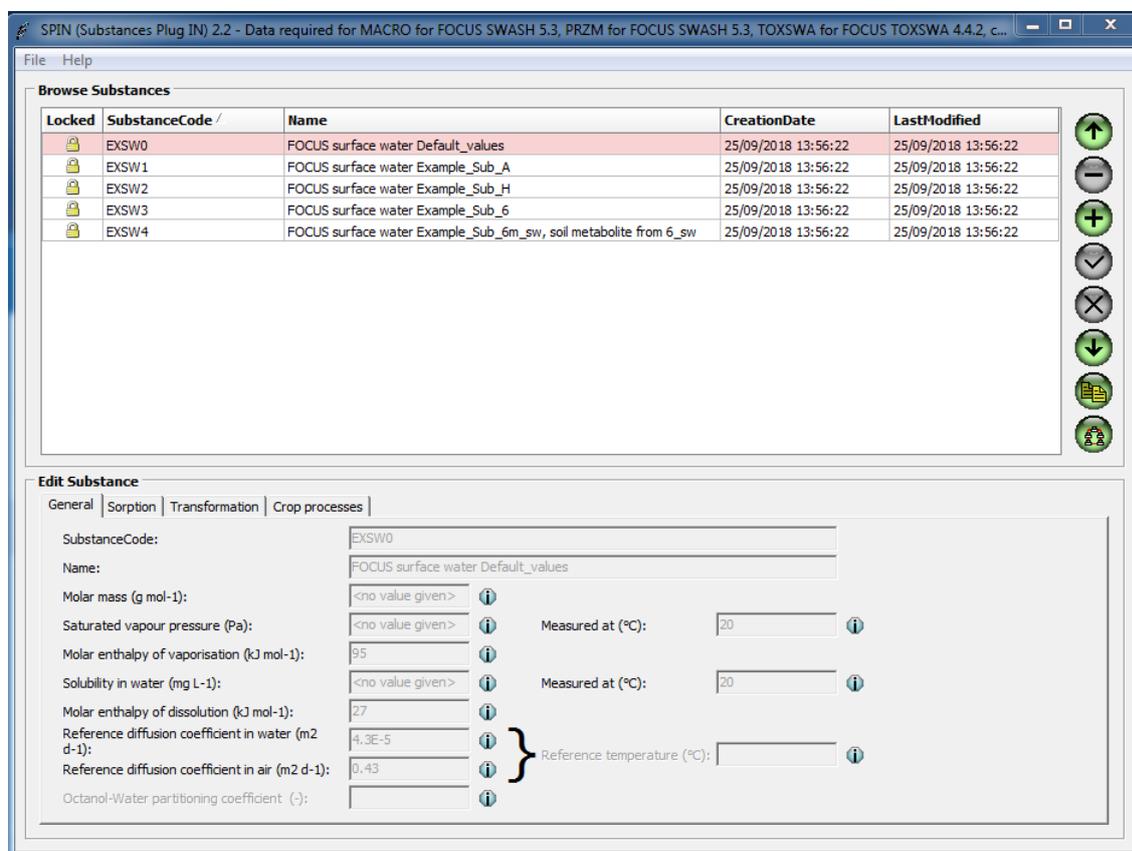


Figure 4.23 View of substances in SPIN database

## 4.10 Editing Application schemes

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

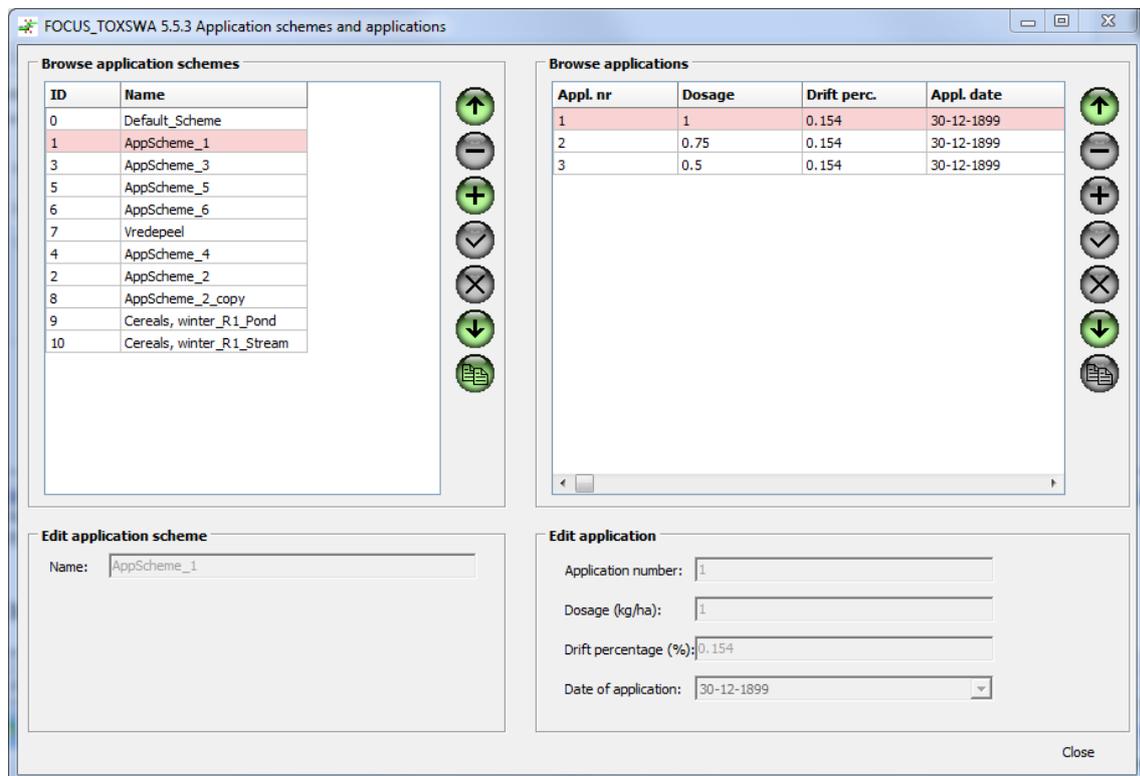
The Application scheme and applications form can be accessed by pressing the  button behind the pick list of the option field 'Application scheme' on the Run Components tab. In the Application Scheme and applications form information about the applications and spray drift can be entered.

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 (including ID) 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 and applications form. The relevant data for drainage and runoff/erosion are entered at the 'Entries' tab of the Runs form.



ID	Name
0	Default_Scheme
1	AppScheme_1
3	AppScheme_3
5	AppScheme_5
6	AppScheme_6
7	Vredepeel
4	AppScheme_4
2	AppScheme_2
8	AppScheme_2_copy
9	Cereals, winter_R1_Pond
10	Cereals, winter_R1_Stream

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 scheme**

Name:

**Edit application**

Application number:

Dosage (kg/ha):

Drift percentage (%):

Date of application:

Figure 4.24 The Application schemes and applications form

The drift percentage may be defined by the user or calculated with the FOCUS drift calculator (Annex 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 schemes and applications form are automatically filled in, because they are defined in SWASH.

---

Note that TOXSWA uses the water depth to convert the mass deposited per  $m^2$  water surface to mass entering per running meter water body, by multiplying the mass deposited per  $m^2$  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 simultaneously on a number of cores of your computer. 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.

### Output options

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.

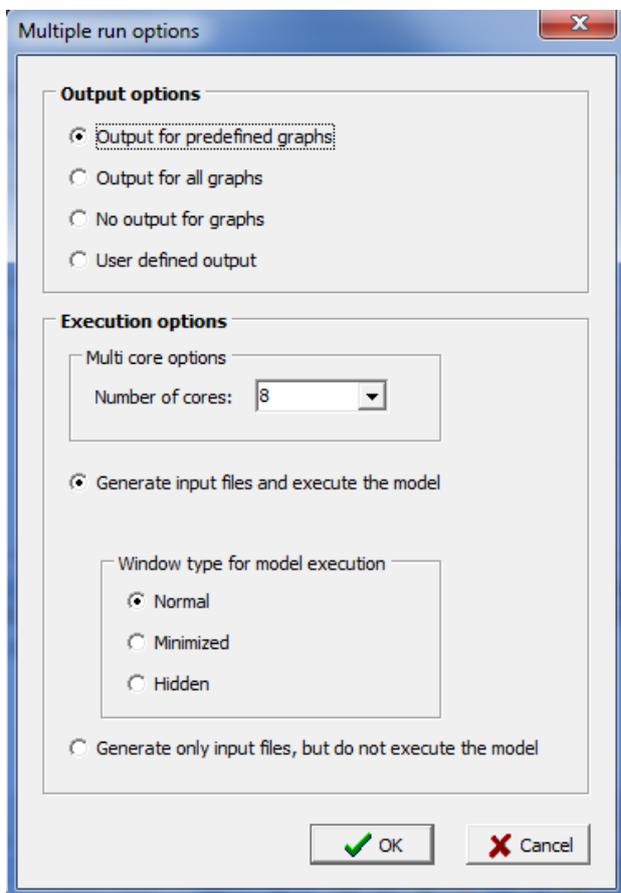


Figure 4.25 Output and execution options offered by TOXSWA when starting a run

### Execution options

The calculations can be executed using the multicore option. Then runs are executed in parallel, each run on a different core of the computer. When the number of runs exceeds the number of cores, the superfluous runs are prepared and appointed to a core that becomes available after having finalized a run. The user can select the number of cores to be used for the simulations, up to the maximum of cores available on the computer. The number of cores available is detected by the GUI. When the user wishes to work on the computer whilst TOXSWA is running, it is advised to select the maximum number of cores minus one because work might be slowed down when all cores are in use.

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.

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 80 seconds on an Intel i7-6700 CPU, 3.40 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 4.7.8. 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).

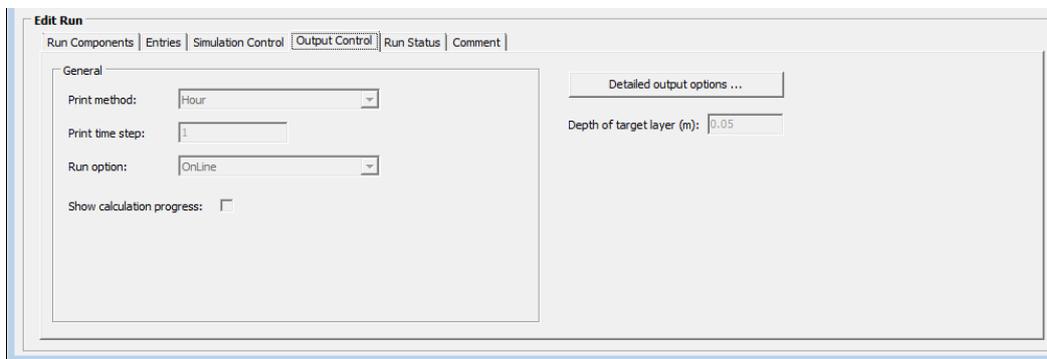


Figure 4.26 The output control tab of the Runs form, with the 'Detailed output options' button on the right side of the tab.

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.

The categories of variables available for output are:

- Hydrology: discharge in water body<sup>10</sup>, 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: balance including e.g. mass in sediment, mass entered from water layer, and mass transformed in sediment.
- 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).

<sup>10</sup> 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.

- 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.

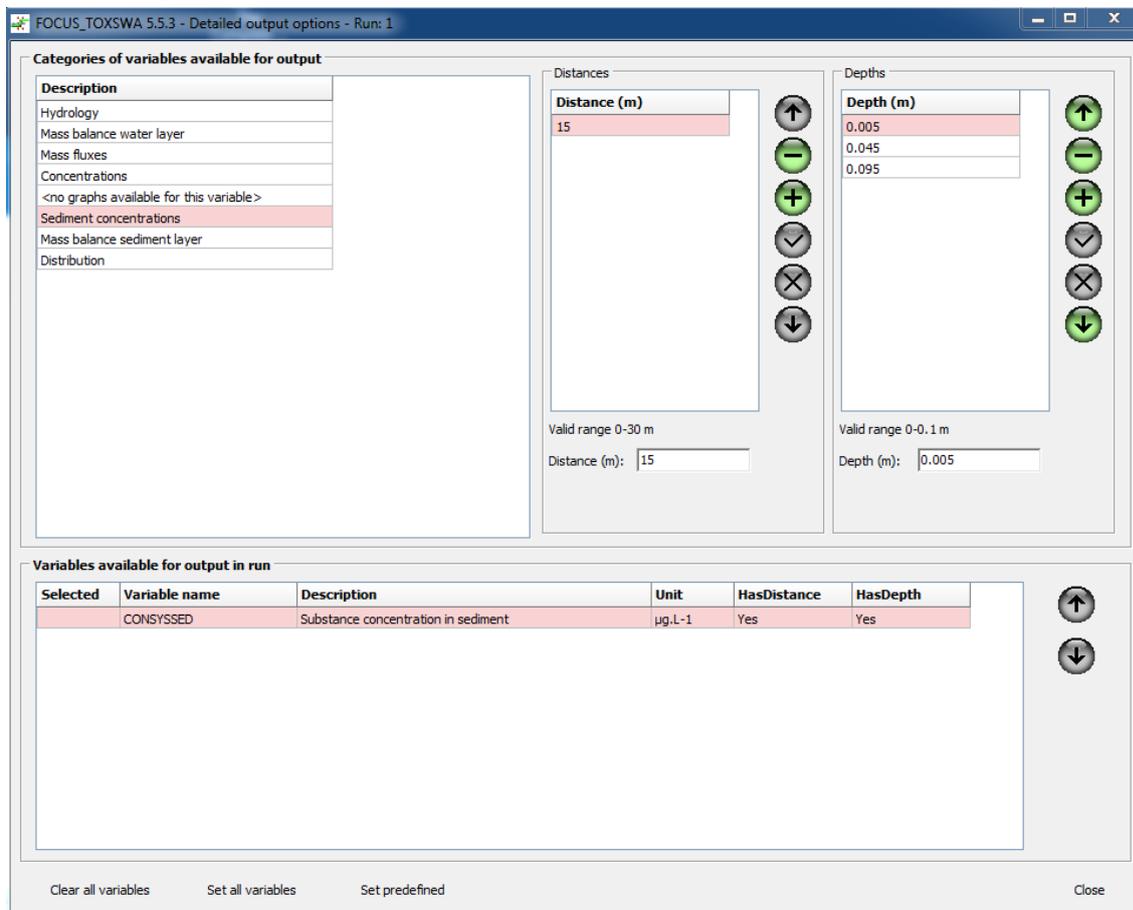


Figure 4.27 The detailed output options form

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 substances for which the graphs are prepared, allowing the user e.g. to choose between a parent substance and one or more of its metabolites. The predefined graphs are accessed through the 'Graphs predefined' button in the Runs form.

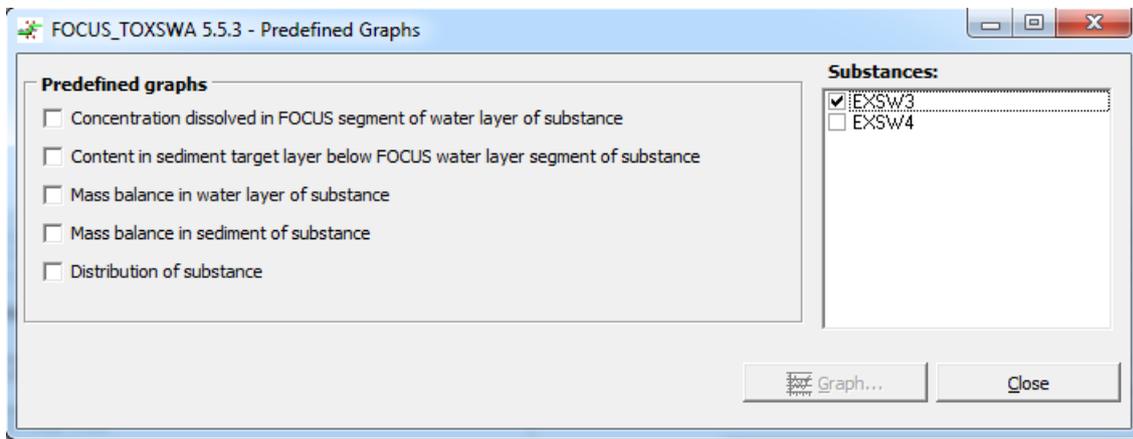


Figure 4.28 Choosing from predefined graphs

#### 4.13.2 User defined graphs

The user is also allowed to create his/her own graphs, enabling him/her 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 5.5.3 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 5.5.3, 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 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,. However if spray drift occurs the concentration at the time – end of the hour- is replaced by the peak concentrations due to spray drift. Otherwise spray drift events would not be visible in the graphs, because spray drift is an instantaneous event.

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.

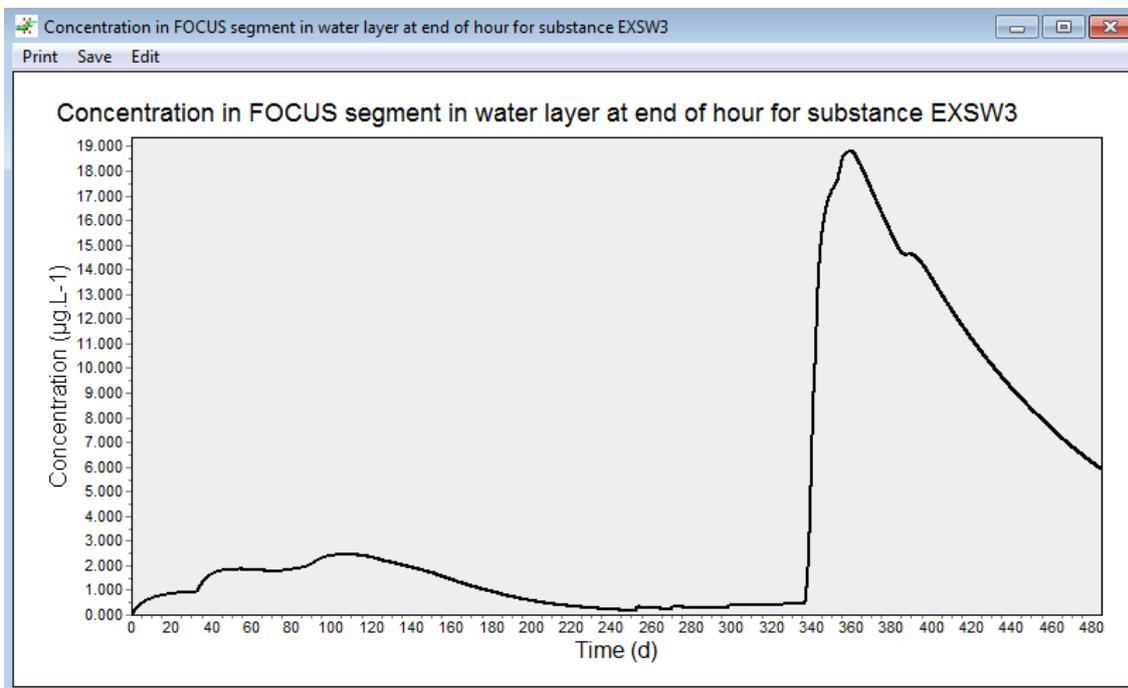


Figure 4.29 TOXSWA graph: Concentration of pesticide in the FOCUS segment of the water layer as a function of time.

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.

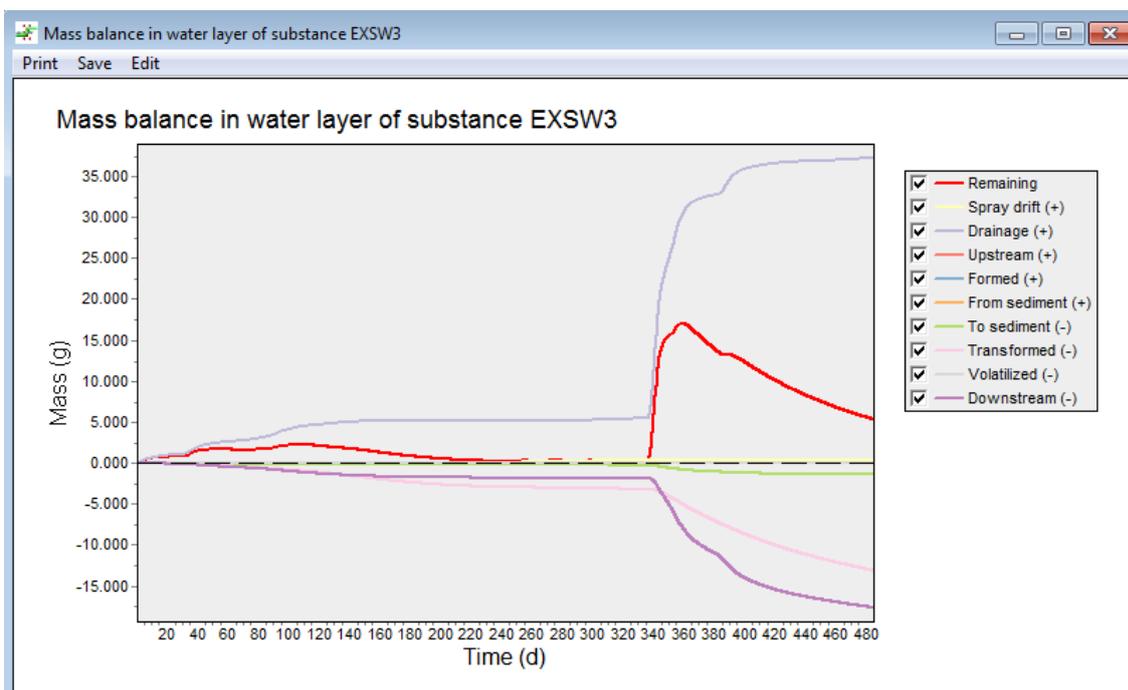


Figure 4.30 TOXSWA graph: Mass balance of pesticide in the water layer as a function of time.

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.

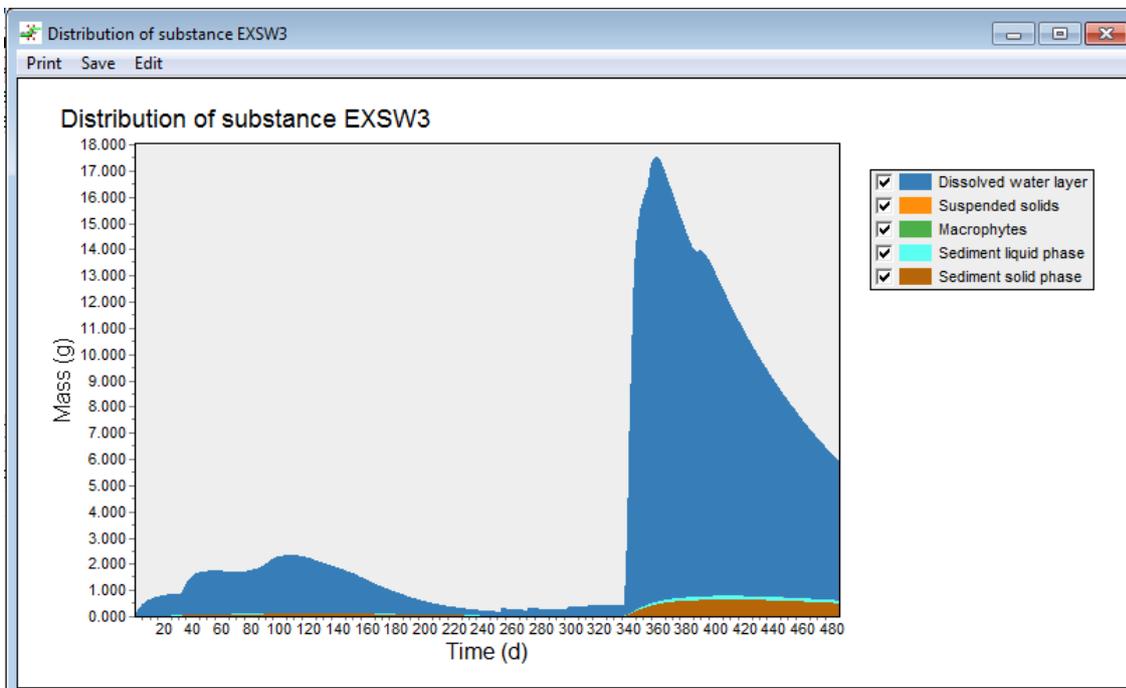


Figure 4.31 TOXSWA graph: Distribution of pesticide over water and sediment compartments as a function of time.

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# 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. Create a project
- b. Create a run
- c. Define the location
- d. Define the substance
- e. Define the application scheme
- f. Specify the 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 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
- 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' (with flow velocity set to zero). 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 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 12 to 14 in Ter Horst *et al.*, 2016). See also the explanation given in Section 3.3.5 for the depth defining perimeter.

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 water-sediment study simulation; they are not used by TOXSWA.

FOCUS\_TOXSWA 5.5.3 - 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 Water Layer**

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

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

**Edit Water Layer**

Name:  Hydrology Type:

General | Watercourse | Pond | **Constant**

Flow velocity (m/s):

Water depth (m):

Dispersion:

Dispersion coefficient (m2/d):

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 can be created. A sediment object consists of several sediment horizons. Each horizon is defined by a number, thickness, a building block and consists of a number of layers. 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 horizons in the right hand side of the form (Figure 5.3).

Because of the bottom up approach in the GUI, Building Blocks needed for the definition of the sediment horizons 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 4.8.3) an existing sediment object must be selected before entering the building blocks form.

**FOCUS\_TOXSWA 5.5.3 Sediment**

**Browse Sediments**

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

**Browse Sediment Horizons**

Horizon no.	Building Block	Thickness	No. of layer
<not available>	<not available>	<not available>	<not available>

**Edit Sediment**

Name:

Description:

Sediment properties:

**Edit Sediment Horizon**

Horizon no.:

Sediment Building Block code:  

Thickness of horizon (m):

No. of layers:

Close

Figure 5.3 The sediment 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 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  $\mu\text{m}$ , based on the particle size class of 105 – 210  $\mu\text{m}$  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 <sup>-3</sup> )	1536
Porosity (-)	0.417
Tortuosity (-)	0.364
Mass ratio of organic matter (kg kg <sup>-1</sup> )	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.

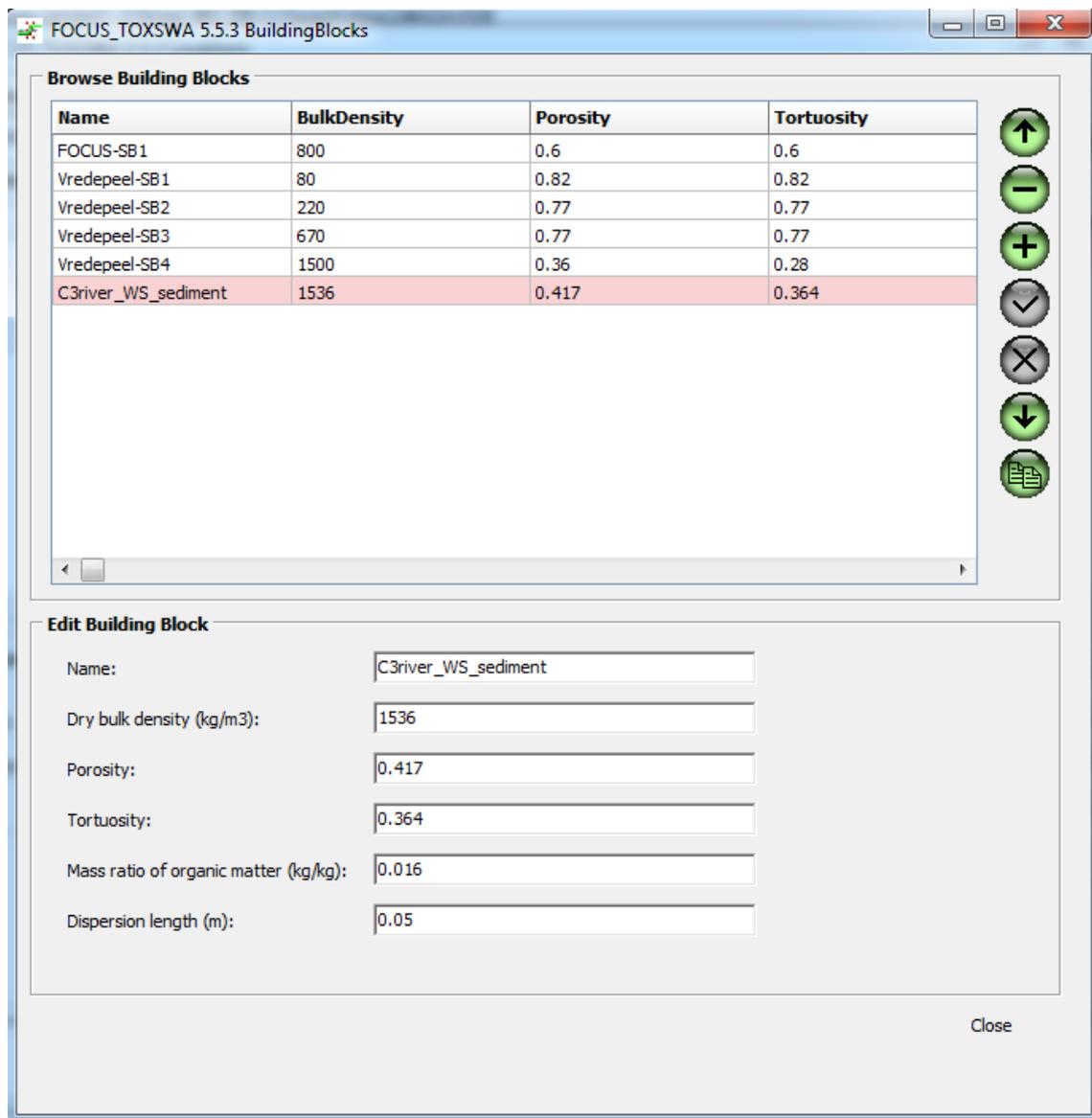


Figure 5.4 The sediment building blocks form for the example water-sediment study

Next the sediment object can be defined by creating new horizons (Figure 5.5). Each horizon contains a building block and consists of a specified number of layers with the same thickness. Note that you need to specify the entire thickness of the horizon. Therefore, a horizon of 0.05 m needs 5 layers to get a thickness of 0.01 m per layer. It is advised to use thin layers of about 0.001 m in the top 0.005 m (0.5 cm) of the sediment. For substances with high  $K_{oc}$  values, the thickness should be even smaller (see Section 4.4.4). Because the  $K_{oc}$  of the example substance is 76 000 L/kg, thin layers have been used. For simplicity, the same segmentation as for the FOCUS-highKoc sediment is used, except for horizon 8, where 3 layers of 0.005 m have been defined instead of 2 layers of 0.005 m. The total thickness of the sediment in the example water-sediment study was 0.025 m. Note that the sediment of the water-sediment study is homogeneous, hence for each horizon the same building block is applied.

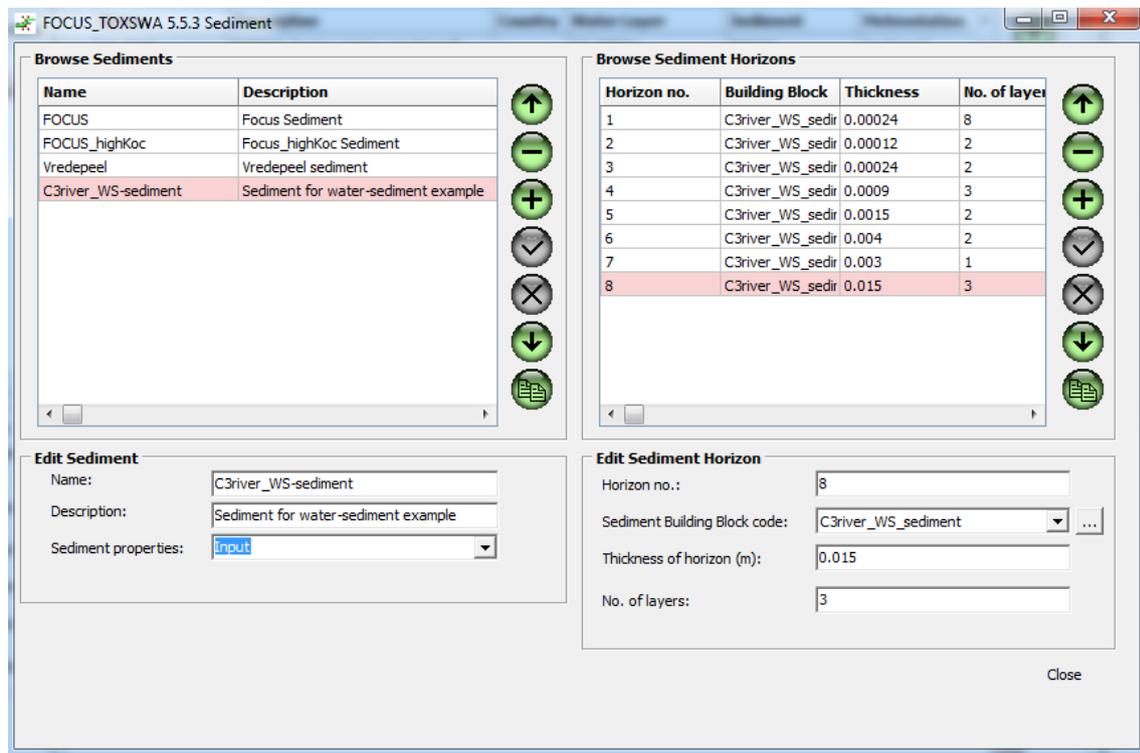


Figure 5.5 Creating a sediment from layers consisting of building blocks

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

### 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).

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 4.8.5). This is also explained in the pop-up box which appears after clicking the button 'Import Datafile...' (Figure 4.22).

```

*
* 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
2000 9 20.00
2000 10 20.00
2000 11 20.00
2000 12 20.00
! - - o^C : unit
! 0 .... 9999 1 .... 12 4. .... 50 : range
*

```

Figure 5.6 Meteorology file of example water-sediment study

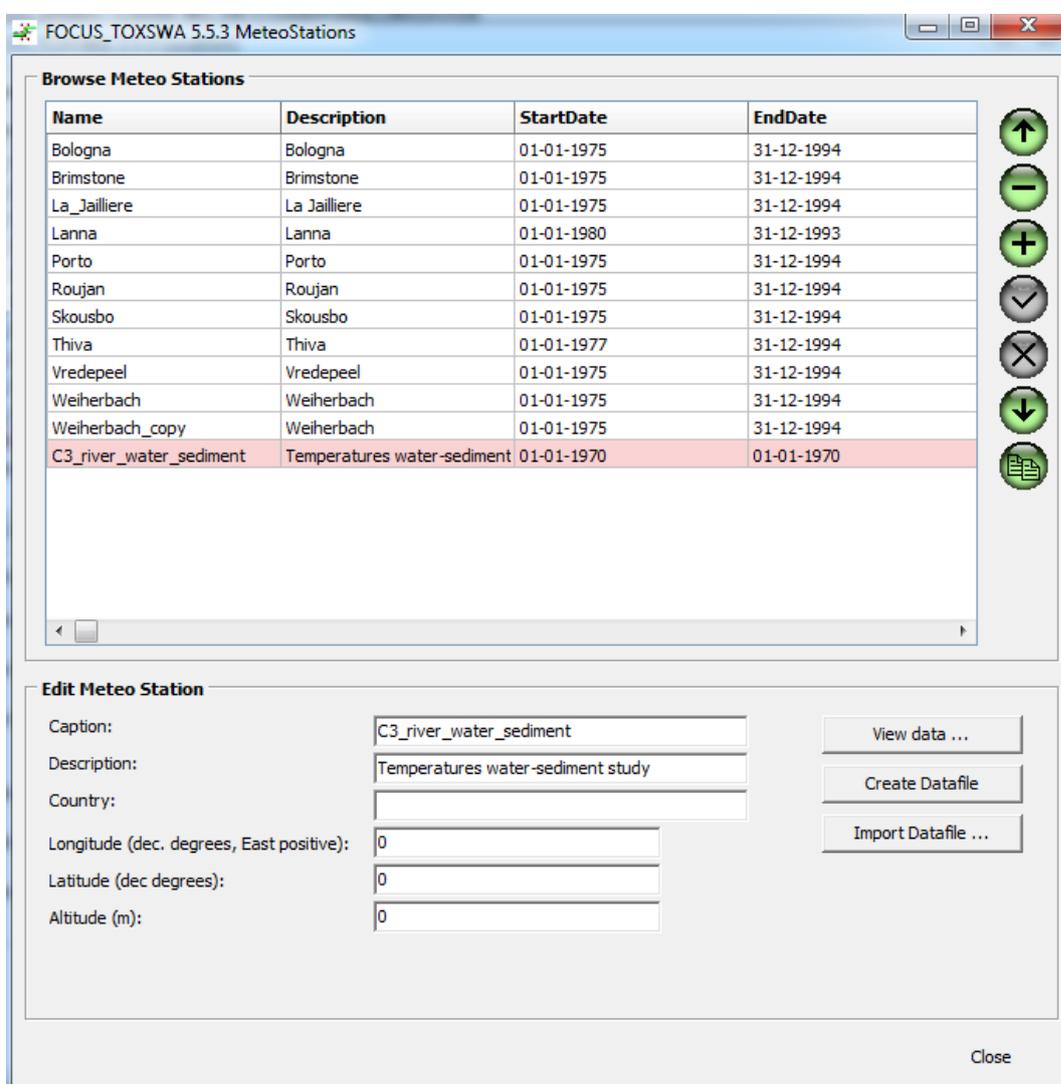


Figure 5.7 Meteo stations form in TOXSWA, enabling the import of a new meteorology data file<sup>11</sup>.

<sup>11</sup> Note that the StartDate and EndDate for the C3\_river\_water\_sediment\_study meteo station are not correct. They should be 01-01-2000 and 31-12-2000, corresponding to the time series in the file. The GUI sets the wrong dates. However, the wrong dates shown in the GUI do not affect proper use of the meteo file. The wrong dates cannot be changed by the user.

## 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).

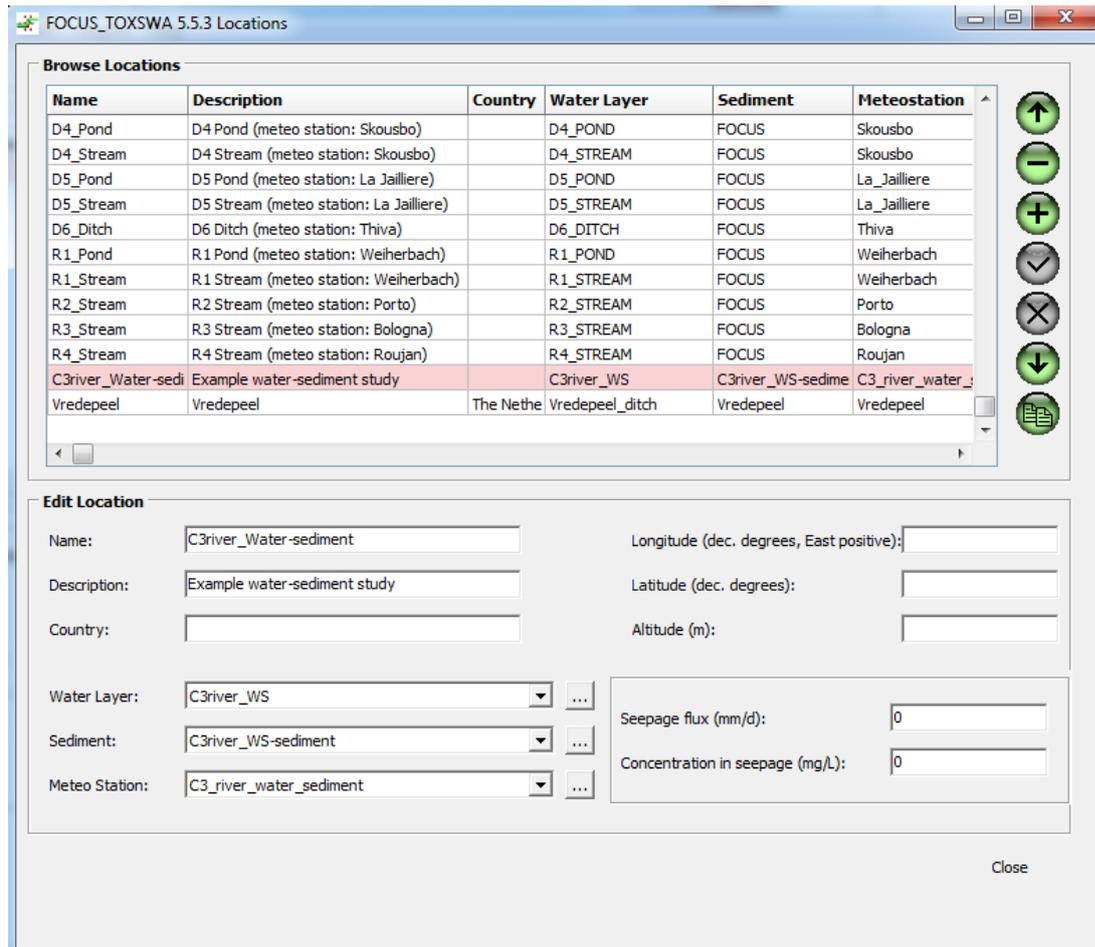


Figure 5.8 The TOXSWA Locations form for the example water-sediment study

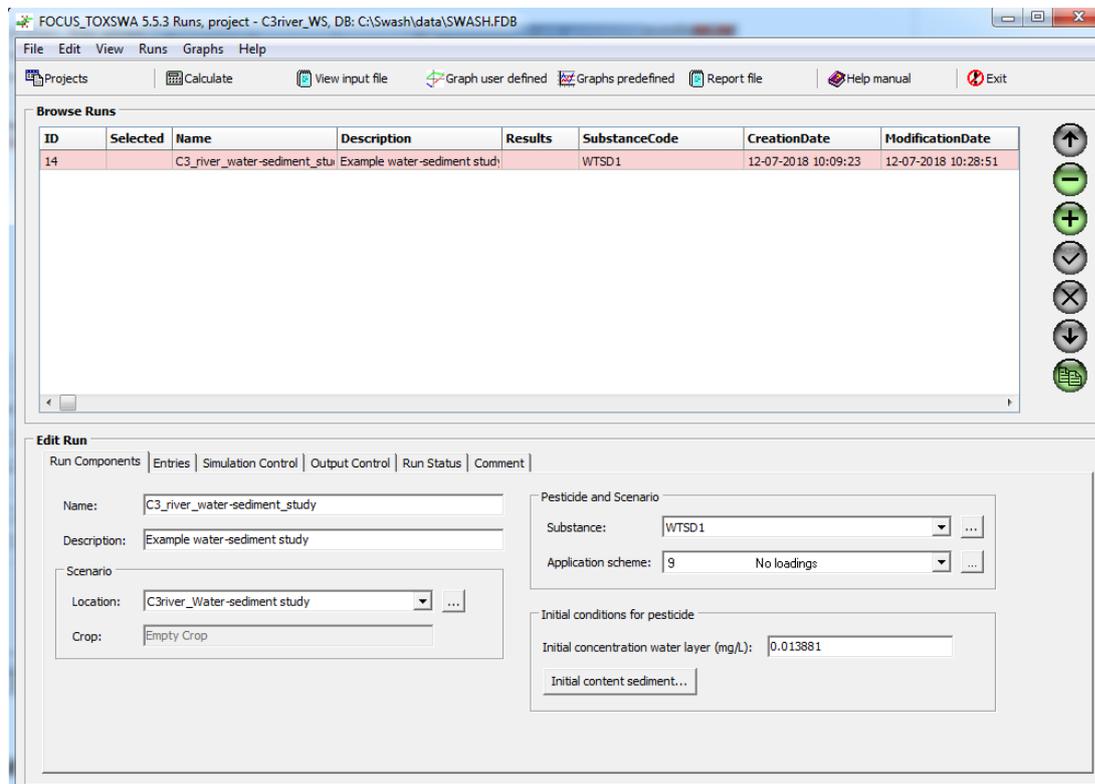


Figure 5.9 The TOXSWA Runs form for the example water-sediment study.

Once the definition of the location for the water-sediment study is 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.

### 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 <sup>-1</sup> )	418.9
Saturated vapour pressure (Pa)	1.7·10 <sup>-7</sup> (20 °C)
Solubility in water (mg L <sup>-1</sup> )	7.5 (25 °C)
K <sub>oc</sub> (L kg <sup>-1</sup> )	76000
Freundlich exponent, <i>N</i> (-)	0.9
DT50 <sub>water</sub> (d <sup>-1</sup> )	0.84 (20 °C)
DT50 <sub>sediment</sub> (d <sup>-1</sup> )	590.0 (20 °C)
Arrhenius activation energy (kJ mol <sup>-1</sup> )	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<sup>-1</sup> resulting in a concentration of 14 µg L<sup>-1</sup> 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<sup>-1</sup>.

---

The water layer consists of one segment (Figure 5.1) so  $13.881 \mu\text{g L}^{-1}$  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<sup>12</sup>

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) and Fate simulation time step. 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. Change the Fate simulation time step. The default option of Calculate combined with 1800 s is too large for the example water-sediment study using a half-life of less than 1 d. Change the Water layer time step option from Calc to Input, and set both time steps to 600 s.

### 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)<sup>13</sup>.

---

<sup>12</sup> When the run with the water-sediment study is started, the run will stop with an error "Missing value OptWaterSystemType". TOXSWA will not do the run. This is a bug. To simulate the water-sediment study we advise to replace FOCUS\_TOXSWA 5.5.3 by the previous version FOCUS\_TOXSWA 4.4.3. This replacement concerns only the GUI and the TOXSWA kernel. Hence the databases remain. Water-sediment runs can then be executed. When later on FOCUS scenarios need to be simulated FOCUS\_TOXSWA 5.5.3 can be set back.

<sup>13</sup> The GUI does not fully support the simulation of the water-sediment study. After having set up the run, export the input file (select "Calculate" and select the option at the bottom "Generate only input files"). Then in a text editor add to the top of the runID.twx file:

```
Pond    OptWaterSystemType
No      OptUpsInp
```

Close the file and run TOXSWA using a batch file (see Section 3.1). The results of the run can be viewed using the GUI.

### 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 ( $\text{g m}^{-3}$ ).

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 ConLiqWatLay, 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 graphs<sup>14</sup>.

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 ( $\text{g m}^{-3}$ )	Residues in sediment (%AR)	Residues in sediment ( $\text{g m}^{-3}$ )
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

<sup>14</sup> The concentrations calculated by TOXSWA can be obtained from the comprehensive \*.out file of TOXSWA, e.g. by using the Sdwin tool (see Appendix 7). Another simple way to obtain the data is via the GUI; plot the predefined graph for concentration in water, select Save from the menu bar 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  $1536 \text{ kg/m}^3$  (Table 5.1).

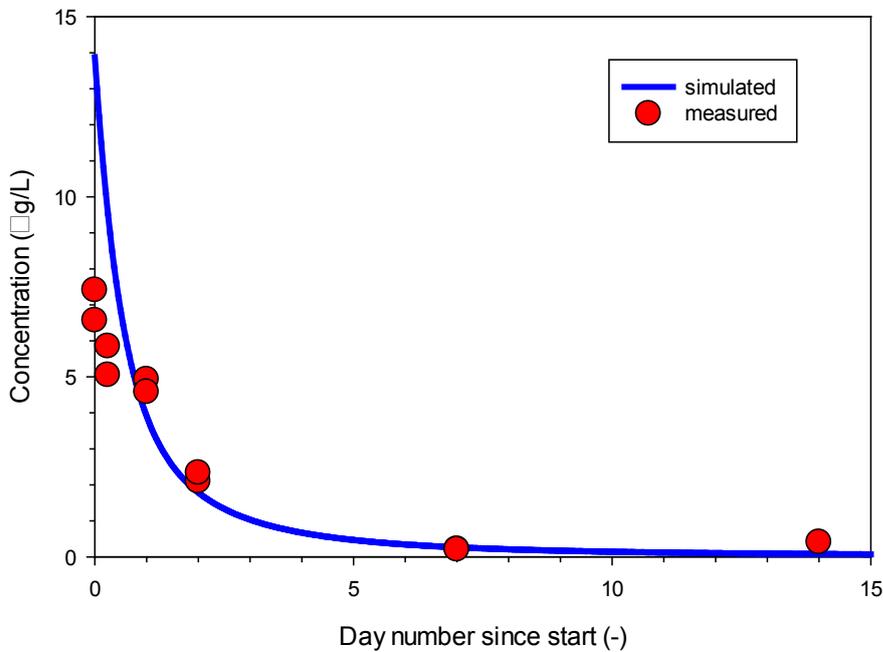


Figure 5.10 Concentration in water for the example water-sediment study; comparison of simulated and measured concentrations.

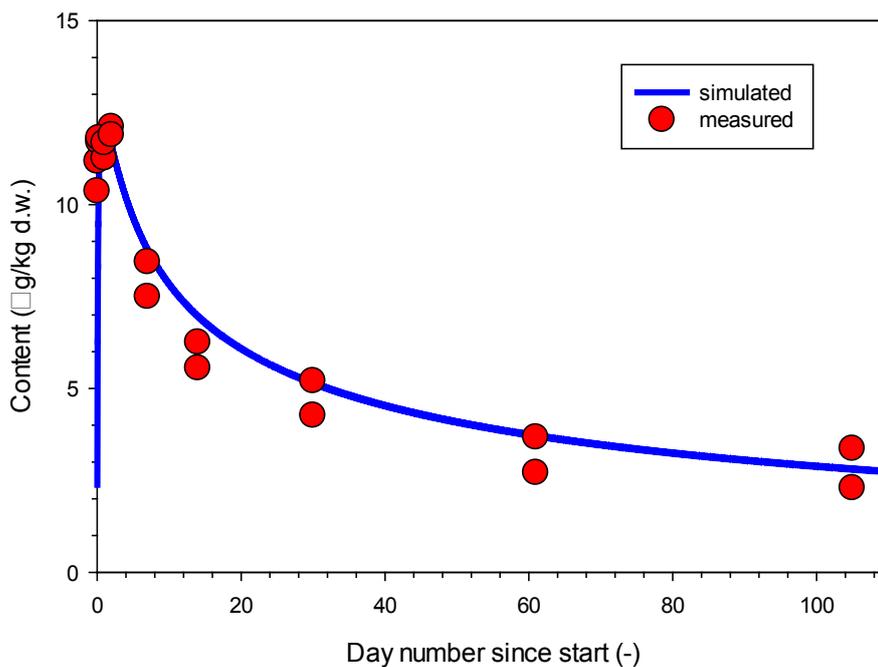


Figure 5.11 Content in sediment for the example water-sediment study; comparison of simulated and measured contents.

---

## 5.2 Multi-year run

### 5.2.1 Introduction

From version 4.4.2 onward FOCUS\_TOXSWA 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 annual maximum 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 the PRZM models for instructions.
- 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 does not have 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 (e.g. Notepad).

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.



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# Justification

This manual is an update of the manual of FOCUS\_TOXSWA 4.4.2 (Beltman *et al.*, 2014). The manual was updated because the TOXSWA kernel, the Graphical User Interface and the database of FOCUS\_TOXSWA were updated.

The project is administered by Jennie van der Kolk (WOT Natuur & Milieu). The project is funded by the Ministry of Agriculture, Nature and Food Quality (project number WOT-04-008-024) with contact person Miranda Meisner.



# Annex 1 FOCUS\_TOXSWA input file for expert users

This Annex lists the extended TOXSWA input file including the legend of the file.

```
*-----
* Input file for TOXSWA
*
* This file is intended to be used by expert users.
*
* E-mail: toxswa@pesticide-models.nl
*
* (c) Wageningen University & Research
*-----

* Section 0: Run identification
* Section 1: Control
* Section 2: Waterbody
* Section 3: Hydrology
* Section 4: Sediment
* Section 5: Weather
* Section 6: Temperature
* Section 7: Substance
* Section 8: Loadings
* Section 9: Initial and boundary conditions for mass balance equations
* Section 10: Output control

* Please note that for scenarios indicated by 'CallingProgram' the following combinations
* are fully tested and supported
* CallingProgram  OptWaterSystemType  OptFloWat  OptReport
* Section 1      Section 3a          Section 3a  Section 10
* 'FOCUS'       'WaterCourse'/'Pond'  'Transient' 'FOCUS'
```

\* Please note that the three following comment lines are given when the txw file is generated by a GUI:

\* This input file considers the current scenario. Input that is not needed for this scenario is omitted. For a description of the full input file, see the user manual for the FOCUS & ascii version or in your TOXSWA download package.

\* Legend of file

- \* \* : on first position of record indicates comment (not read by TOXSWA)
- \* a : obligatory parameter values are given from first position of record onwards
- \* a : parameter values not obligatory for running TOXSWA are given from fifth or ninth position of record (these positions create a clear layout of this txw input file, however, TOXSWA does not discriminate between these two types of position)
- \* (units) : units between brackets (one space between units and "!" obligatory to avoid crashes)
- \* ! : text behind is comment
- \* [a, b] : entries a and b are words: two options, can be extended with more options
- \* [a|b] : entries a and b are values: a = minimum, b = maximum;
- \* empty positions indicates no minimum and maximum values exist
- \* table : start of table
- \* table horizon : start of table in which properties are given per horizon, using the horizon definitions given in the SedimentProfile table as a key
- \* table interpolate : start of table with values are given that are linearly interpolated onto the nodes given in the SedimentProfile table by TOXSWA
- \* end\_table : end of table (note that a table can be empty)
- \* e-10 : example format for exponential values
- \* 'table' : option for output indicating that the output can be obtained in a table for selected nodes
- \* 'Input' : option indicating that a parameter is user input
- \* 'Calc' : option indicating that a parameter is calculated by TOXSWA

\* Description of general characteristics of file

- \* - numerical records consist of an input field (field 1), an identifier (field 2), an optional dimension field (field 3), and a comment field (remainder of record), e.g.:
- \* 900 TimStpHyd (s) ! Calculation time step for hydrology [0.001|3600]
- \* - Option records consist of the input field (field 1), an identifier (field 2) and a comment field (remainder of record), e.g.:
- \* Hourly OptInp ! Option for hourly or daily input data of lateral entries [Hourly|Daily]
- \* - date and time formats acceptable for TOXSWA are: d-mmm-yyyy, dd-mmm-yyyy, dd-mmm-yyyy-hhmm, dd-mmm-yyyy-hh-mm, dd-mmm, dd/mmm/yyyy
- \* - integer and real values can be entered, unless the parameter is indisputably an integer, e.g. number of segments, or it is indicated that an integer is requested
- \* - default values for parameters are not applied by TOXSWA, except when explicitly indicated in this txw file

```
*-----
* Section 0: Run identification
*-----

R1_Stream      Location          ! Name of the location [1|25 characters]
R1_Stream      WaterbodyID      ! ID of the water body [1|25 characters]
FOCUS          SedimentTypeID   ! Name of sediment type [1|25 characters]
EXSW2          SubstanceName    ! Name of parent substance [1|15 characters]
EXSW2-maize    ApplicationScheme ! Name of the application scheme [1|25 characters]
```

```

*-----
*-----
* Section 1: Control
*-----
FOCUS      CallingProgram      ! Release type of scenario [FOCUS]
5.5.3      CallingProgramVersion ! Version numbers for model, interface and database,
           ! respectively

01-Oct-1978 TimStart      ! Starting time of simulation [01-Jan-1900|31-Dec-9999]
30-Sep-1979 TimEnd       ! End time of simulation [01-Jan-1900|31-Dec-9999]

Hourly     OptInp         ! Option for hourly or daily input data of lateral entries [Hourly, Daily]

* OptHyd: options for hydrology simulation
* Only     Simulate only hydrology
* OnLine   Simulate hydrology and substance
* OffLine  Assumption hydrology has been simulated, runID.hyd file must be present
* Automatic TOXSWA checks if hydrology file (runID.hyd) exists; so, hydrology
           simulation is skipped
Automatic  OptHyd        ! Option selected for hydrology simulation
           ! [Only, OnLine, OffLine, Automatic]
600       TimStpHyd (s)   ! Calculation time step for hydrology [0.001|3600]

* OptTem: options for temperature simulation
* Only     Simulate only temperature
* OnLine   Simulate temperature and substance
* OffLine  Assumption temperature has been simulated, runID.tem file must be present
* Automatic TOXSWA checks if the temperature file (runID.tem) exists; so, temperature
           simulation is skipped
OnLine     OptTem        ! Option selected for temperature simulation
           ! [Only, OnLine, OffLine, Automatic, ExtModel]

Calc       OptTimStp     ! Option for time step in mass balance calculation [Input, Calc]
Yes        OptCalcStabilityWater ! Option for check of stability of the numerical solution for
           ! the water layer
Yes        OptCalcStabilitySediment ! Option for check of stability of the numerical solution for
           ! the sediment [Yes, No]
           ! Yes = Full check on stability
           ! No = Check on positivity

* If OptTimStp is 'Input' then specify
600       TimStpWat (s)   ! Calculation time step in water layer [0.001|3600]
600       TimStpSed (s)  ! Calculation time step in sediment [0.001|3600]

* If OptTimStp is 'Calc' then specify
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]

*-----
*-----
* Section 2: Waterbody
*-----
* WaterBody table: description of waterbody
* Len      Length [0.05|]
* NumSeg   Number of segments [1|]
* WidWatSys Width of the bottom of water system [0.05|100]
* SloSidWatSys Side slope of the water system [0|10]
* DepWatDefPer Water depth defining perimeter for exchange between water layer
*           and sediment [0|lowest water depth]
table WaterBody
Len  NumSeg  WidWatSys  SloSidWatSys  DepWatDefPer
(m)  (-)     (m)         (-)           (m)
100  20      1           1.E-5         0.01
end_table

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

*-----
*-----
* Section 3: Hydrology:
* Section 3a: General
*-----
Transient OptFloWat      ! Water flow type [Constant, Transient]
WaterCourse OptWaterSystemType ! Water system type [Pond, WaterCourse]

* If OptWaterSystemType is 'WaterCourse' then specify
Fischer   OptDis        ! Dispersion calculation method [Input, Fischer]

* If OptDis is 'Input' then specify
600      CofDisPhsInp (m2.d-1) ! Dispersion coefficient [0|1e6]

*-----
* Section 3b: Constant water flow
*-----
* If OptFloWat is 'Constant'

```

```

*-----
1          DepWat (m)          ! Water depth [0.001|10]
100       VelWatFlwBas (m.d-1) ! Flow velocity [-1e5|1e5]

*-----
* Section 3c: Variable flow: pond
*
* If OptFloWat is 'Transient' and OptWaterSystemType is 'Pond'
*-----

0.45     AreaSurPndInp (ha ) ! Size of surrounding area discharging excess water into the pond
          ! [0|100]
3.189    QBasPndInp (m3.d-1) ! Base flow, i.e. inflow into pond [0|50]
0.5      HgtCrePnd (m)       ! Height of the weir crest at outflow [0.1|5]
0.5      WidCrePnd (m)       ! Width of the weir crest at outflow [0.01|10]

      * If application option OptLoa is 'PRZM' then specify
      0.06 AreaErsSurPndInp (ha) ! Size of the eroding area around the pond [0|100]

*-----
* Section 3d: Variable flow: watercourse
*
* If OptFloWat is 'Transient' and OptWaterSystemType is 'WaterCourse'
*-----

100      AreaUpsWatCrSInp (ha) ! Area of upstream catchment [0|1e4]
191.8    QBasWatCrSInp (m3.d-1) ! Base flow from upstream catchment [0|1e4]
0.001    SloBotRepCha (-)      ! Slope bottom representative channel [0|0.01]
0.5      HgtCreRepCha (m)      ! Height of the weir crest [0.01|5]
0.5      WidCreRepCha (m)      ! Width of the weir crest [0.01|10]
110      LenRepCha (m)         ! Length representative channel [10|2000]
11       CofRghRef (s-1)       ! Value Manning coefficient for bottom roughness at 1 m
          ! water depth in water body [1|100]
1.2      CofVelHea (m.s-1)     ! Energy coefficient due to non-uniform distribution of
          ! flow velocities in cross section [1.1|1.5]

*-----
* Section 4: Sediment
*
* SedimentProfile table: thickness and number of layers in horizon
* ThiHor Thickness of horizon [0.0001|-]
* NumLay Number of layers in horizon [1|500]
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 ! Sediment properties for ThetaSat and CofDifRel [Input, Calc]

* SedimentProperties table: properties for each horizon:
* Nr Number horizon [1|500]
* Rho Bulk density [10|3000]
* CntOm Organic matter mass content [0|1]
* If OptSedProperties 'Input' then specify ThetaSat and CofDifRel
* ThetaSat Saturated water content [0.001|0.999]
* CofDifRel Relative diffusion coefficient [0|1]
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) ! Percolation rate through the sediment [-0.01|0.01]

* DispersionLength table: dispersion length for each horizon
* Nr Horizon number [1|500]
* LenDisSedLiq Dispersion length of solute in liquid phase (m) [0.01|1]
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

```

```

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

Weierbach   MeteoStation   ! Name of file with meteo data (*.met)
Monthly     OptMetInp      ! Input data [Monthly]

-----

* Section 6: Temperature

-----

* Section 7: Substance
* Section 7a: general
-----

* Compounds table: first entry is parent, next entries are metabolites [1|15 characters]
table compounds
EXSW2
end_table

* FraPrtDauWat table: parent-daughter relationships transformation in water
* Column 1: fraction formed from parent into daughter [0|]
* Column 2: name of parent
* Column 3: name of daughter
table FraPrtDauWat (mol.mol-1)
end_table

* FraPrtDauSed table: parent-daughter relationships transformation in sediment
* Column 1: fraction formed from parent into daughter [0|]
* Column 2: name of parent
* Column 3: name of daughter
table FraPrtDauSed (mol.mol-1)
end_table

-----
* Section 7b: Substance properties for parent 'EXSW2'
* (note extension of parameter name is substance code)
-----

300          MolMas_EXSW2 (g.mol-1)      ! Molar mass [10|10000]

* Volatilization from water layer
1.E-4        PreVapRef_EXSW2 (Pa)      ! Saturated vapour pressure of substance [0|2e5]
20           TemRefVap_EXSW2 (C)      ! Reference temperature for saturated vapour pressure
! [0|40]
95.          MolEntVap_EXSW2 (kJ.mol-1) ! Molar enthalpy of vaporization [-200|200]
1            SlbWatRef_EXSW2 (mg.L-1)  ! Water solubility of substance [0.001|1e6]
20           TemRefSlb_EXSW2 (C)      ! Reference temperature for water solubility [0|40]
27           MolEntSlb_EXSW2 (kJ.mol-1) ! Molar enthalpy of dissolution [-200|200]

* Diffusion in liquid phase
4.3E-5       CofDifWatRef_EXSW2 (m2.d-1) ! Reference diffusion coefficient in water [0|2E-3]

* Sorption
58           KomSed_EXSW2 (L.kg-1)     ! Freundlich coefficient of equilibrium sorption for
! sediment [0|1e7]
1            ConLiqRefSed_EXSW2 (mg.L-1) ! Reference concentration in liquid phase for
! Freundlich coefficient for sediment [0.001|100]
1            ExpFreSed_EXSW2 (-)       ! Freundlich exponent in sediment [0.1|1.5]
58           KomSusSol_EXSW2 (L.kg-1)  ! Freundlich coefficient of equilibrium sorption
! for suspended solids [0|1e7]
1            ConLiqRefSusSol_EXSW2 (mg.L-1) ! Reference concentration in liquid phase
! for Freundlich sorption coefficient for
! suspended solids [0.001|100]
1            ExpFreSusSol_EXSW2 (-)    ! Freundlich exponent suspended solids [0.1|1.5]
0            CofSorMph_EXSW2 (L.kg-1)  ! Coefficient for linear sorption on
! macrophytes [0|1e7]

* Transformation in water
2            DT50WatRef_EXSW2 (d)      ! Half-life transformation in water at reference
! temperature [0.1|1e5]
20           TemRefTraWat_EXSW2 (C)    ! Reference temperature for half-life measured in
! water [5|30]
65.4        MolEntTraWat_EXSW2 (kJ.mol-1) ! Molar activation enthalpy of transformation in
! water [0|200]

* Transformation in sediment
3            DT50SedRef_EXSW2 (d)      ! Half-life transformation in sediment at reference
! temperature [0.1|1e5]
20           TemRefTraSed_EXSW2 (C)    ! Reference temperature for half-life in sediment
! [5|30]
65.4        MolEntTraSed_EXSW2 (kJ.mol-1) ! Molar activation enthalpy of transformation in
! sediment [0|200]

```

```

*-----
* Section 7c: Substance properties for metabolite MetW1
*-----

*-----
* Section 8: Loadings
*-----

* OptLoa options for loading type
* DriftOnly spray drift only entry route
* MACRO drainage calculated by MACRO
* PRZM runoff and erosion calculated by PRZM
PRZM OptLoa ! Loading option [DriftOnly, PEARL, MACRO, PRZM, GEM]

* Loadings table: details on spray drift, and stretch for all loading types
* Column 1 Date and time of application, relevant if OptLoa is 'DriftOnly', otherwise
* the date is a dummy value
* Column 2 Type of loading [Drift]
* Column 3 Drift deposition (mg.m-2) [0]
* Column 4 Start of stretch of watercourse loaded by all loading types (m) [0|1e4]
* Column 5 End of stretch of watercourse loaded by all loading types (m) [0|1e4]
table Loadings
31-Dec-1899-09h00 Drift 1.716 0 100
end_table

* If OptLoa is 'MACRO' then specify details of drainage
100 WidFldDra (m) ! Width of field contributing drainage [0|1000]

* If OptLoa is 'PRZM' then specify details of runoff
100 WidFldRnf (m) ! Width of field contributing runoff [0|1000]
20 WidFldErs (m) ! Width of field contributing erosion [0|1000]
0.1 RatInfDir (-) ! Ratio of infiltration water added to runoff water [0|1]
0.01 ThiLayErs (m) ! Thickness of upper sediment layer to which erosion mass
! is added [1e-5|1]

* If OptLoa is 'MACRO' or OptLoa is 'PRZM' then specify path and file names of files
* Table lateral entries files of soil substances, including metabolites (path+name)
Table Soil Substances
00003-C1.p2t
end_table

* If OptHyd is 'transient' then specify details of catchment
Yes OptUpsInp ! Upstream catchment treated [Yes, No]
0.2 RatAreaUpsApp (-) ! Ratio of upstream catchment treated [0|1]

* If metabolite formed in water then
0.013 FraMetForUps_MetW1 (-) ! Fraction metabolite formed in water in upstream
! catchment [0|1]

*-----
* Section 9: Initial and boundary conditions for mass balance equations
*-----

* Initial conditions

0 ConSysWatIni (g.m-3) ! Initial total concentration in water layer [0|-]

* CntSysSedIni table: initial total substance content in sediment
* If metabolites are included then initial contents for these substances are set to zero
* Column 1 Depth in sediment (m) [0|-]
* Column 2 Substance content (mg.kg-1) [0|-]
table interpolate CntSysSedIni (mg.kg-1)
end_table

* Boundary conditions

0 ConAir (g.m-3) ! Concentration in air [0|-]

0 ConWatSpq (g.m-3) ! Concentration in incoming seepage water [0|-]

*-----
* Section 10: Output control
* Section 10a: General
*-----

No OptDelOutFiles ! Remove *.out file after simulation [Yes|No]

* DateFormat: options for format of date and time in the output file
* DaysFromSta Print number of days since start of simulation
* DaysFrom1900 Print number of days since 1900
* Years Print years
DaysFromSta DateFormat [DaysFromSta, DaysFrom1900, Years]

* RealFormat: format of the ordinary output - use FORTRAN notation:
* e is scientific notation, g is general notation,
* then the number of positions, then the number of digits
e14.6 RealFormat ! Format of ordinary output

```

```

* OptDelTimPrn: options for output time step
* Hour,Day,Decade,Month,Year Time step for output
* Automatic Length of simulation period
* Other User defined
Hour OptDelTimPrn ! Output time step [Hour|Day|Decade|Month|Year|
! Automatic|Other]

* If OptDelTimPrn is 'Other' then specify
5 DelTimPrn (d) ! Output time step [1|length simulation period]
! Integer value required

0.05 ThiLayTgt (m) ! Depth defining the thickness of the target sediment layer
! for output of (averaged) content [1e-5|1]

table OptOutputDistances ! Options for distances of water layer grid points at which
! output can be obtained[None, All, table]

* If OptOutputDistances is 'table' then specify output distances in waterbody
* OutputDistances-table: output distances in waterbody, i.e. water layer and sediment
* subsystem
* Column 1 Distance (m) [0|-]
table OutputDistances (m)
97.5
end_table

table OptOutputDepths ! Options for depths of sediment grid points at which
! output can be obtained [None, All, table]

* If OptOutputDepths is 'table' then specify
* OutputDepths-table: depths of sediment nodes at which output can be obtained
* Column 1 Depth (m) [0|-]
table OutputDepths (m)
0.003
0.05
end_table

* Specify dates for output of additional profiles; options set via OptOutputDistances and
* OptOutputDepths are used
* HorVertProfiles table: profiles in horizontal direction for water layer and in vertical
* direction for sediment are given; values given are:
* Water layer: output distance, water depth, total and dissolved concentration,
* Sediment: output node water layer, output depth, pore volume, total and dissolved
* concentration.
table HorVertProfiles
end_table

* Specify type of summary report
FOCUS OptReport ! [FOCUS]
Yes ExposureReport ! Exposure report [Yes|No]

-----
* Section 10b: Additional options for Dutch registration report
*
* If OptReport is 'DutchRegistration'
*-----

-----
* Section 10c: Print variables in *.out file
* State variables, fluxes and rates given as momentary values.
* Volume, energy and mass changes given as cumulative values.
*-----

* Specify for all print variables whether output is wanted [Yes, No]
* When print variable is not in file; TOXSWA assumes 'No'

* PrintCumulatives: options for printing cumulatives of volume, energy and mass fluxes
* Yes : cumulative terms have been summed up from start of simulation and have been
* allocated to the last moment of the period considered
* No : cumulative terms have been summed up from start of user defined output time step
* OptDelTimPrn and have been allocated to the last moment of the period
* considered
Yes PrintCumulatives ! [Yes, No]

* Hydrology
Yes print_DepWat ! Water depth (m)
Yes print_QBou ! Discharge (m3.s-1)
Yes print_VelWatFlw ! Flow velocity (m.d-1)
Yes print_VolErrWatLay ! Volume error in waterbody (m3)

* Lateral entries (expressed per m2 adjacent field)
* If OptLoa is 'MACRO'
Yes print_VvrLiqDra ! Drain flow (m3.m-2.hr-1)
Yes print_FlmDra ! Drain substance flux (g.m-2.hr-1)
* If OptLoa is 'PRZM'
Yes print_VvrLiqRnf ! Runoff (+ infiltration) water flow (m3.m-2.hr-1)
Yes print_FlmRnf ! Runoff substance flux (g.m-2.hr-1)
Yes print_FlmErs ! Erosion substance flux (g.m-2.hr-1)

* Concentrations and contents in water layer segments as specified by
* OptOutputDistances
Yes print_ConLiqWatLay ! Concentration dissolved in water (g.m-3)
No print_CntSorMph ! Content sorbed to macrophytes (g.kg-1)
No print_CntSorSusSol ! Content sorbed to suspended solids (g.kg-1)

```

```

No      print_ConSysWatLay    ! Total concentration in water (g.m-3)

* Concentrations and contents in sediment below water layer segments as specified by
* OptOutputDistances and OptOutputDepths
Yes     print_ConLiqSed      ! Concentration in pore water sediment (g.m-3)
No      print_CntSorSed      ! Content sorbed to sediment (g.kg-1)
No      print_ConSysSed      ! Total content in sediment (g.m-3)
No      print_CntSedTgt      ! Total content in target layer sediment (g.kg-1)
Yes     print_ConLiqSedTgt   ! Concentration in pore water in target layer
                                           ! sediment (g.m-3)
No      print_CntSorSedTgt   ! Content sorbed in target layer sediment (g.kg-1)

* Distribution in entire water layer
Yes     print_MasLiqWatLay    ! Mass in liquid phase in water layer (g)
Yes     print_MasSorSusSol    ! Mass sorbed to suspended solids in water layer (g)
Yes     print_MasSorMph       ! Mass sorbed to macrophytes in water layer (g)

* Distribution in entire sediment
Yes     print_MasLiqSed      ! Mass in liquid phase in sediment (g)
Yes     print_MasSorSed      ! Mass sorbed in sediment (g)

* Mass balance for entire water layer
Yes     print_MasWatLay      ! Mass in water layer (g)
Yes     print_MasDrfWatLay   ! Mass entered in water layer by spray drift (g)
Yes     print_MasDraWatLay   ! Mass entered in water layer by drainage (g)
Yes     print_MasRnoWatLay   ! Mass entered in water layer by runoff (g)
Yes     print_MasSedInWatLay ! Mass penetrated into sediment from water layer (g)
Yes     print_MasSedOutWatLay ! Mass transferred from sediment into water layer (g)
Yes     print_MasDwnWatLay   ! Mass flowed across downstream boundary out of
                                           ! water layer (g)
Yes     print_MasUpsWatLay   ! Mass flowed across upstream boundary into water
                                           ! layer (g)
Yes     print_MasTraWatLay   ! Mass transformed in water layer (g)
Yes     print_MasForWatLay   ! Mass formed in water layer (g)
Yes     print_MasVolWatLay   ! Mass volatilised from water layer (g)
Yes     print_MasErrWatLay   ! Mass error in water layer (g)

* Mass balance sediment
Yes     print_MasSed         ! Mass in sediment (g)
Yes     print_MasTraSed      ! Mass transformed in sediment (g)
Yes     print_MasForSed      ! Mass formed in sediment (g)
Yes     print_MasWatLayInSed ! Mass transferred into water layer from sediment
                                           ! layer (g)
Yes     print_MasWatLayOutSed ! Mass transferred from water layer into sediment
                                           ! layer (g)
Yes     print_MasDwnSed      ! Mass leaving sediment across lower boundary (g)
Yes     print_MasErsSed      ! Mass entering sediment by erosion (g)
Yes     print_MasErrSed      ! Mass error in sediment (g)

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

```

## Annex 2 Technical description of the TOXSWA input file

### Legend to table:

ID	Name of parameter or variable in file
Units	Units
Single/Array	Single value, used for entire water body, or array of values, attributed to distance in water layer or depth in sediment
Array delimitation	Array: maximum number of values
Substance specific	Parameter or variable is substance specific
Has distance	Parameter of Variable attributed to distance in water layer
Has depth	Parameter of variable attributed to depth in sediment
Limits on value	Boundaries for values or options
Description	Description
Comment	Comment

ID	Units	Single/Array	Array delimitation	Substance specific	Has distance	Has depth	Limits on value	Description	Comment
Section 0									
Location	-	S	1	N	N	N	1-25 characters	Name of the location	
WaterbodyID	-	S	1	N	N	N	1-25 characters	ID of the water body	
SedimentTypeID	-	S	1	N	N	N	1-25 characters	Name of sediment type	
SubstanceName	-	S	1	Y	N	N	1-15 characters	Name of parent substance	
ApplicationScheme	-	S	1	N	N	N	1-25 characters	Name of the applicaton scheme	

ID	Units	Single /Array	Array delimitation	Substance specific	Has distance	Has depth	Limits on value	Description	Comment
Section 1									
CallingProgram	-	S	1	N	N	N	FOCUS	Release type of scenario	
CallingProgramVersion	-	S	1	N	N	N	integer.integer.integer	Version numbers (model.GUI.database)	
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	
OptInp	-	S	1	N	N	N	Hourly,Daily	Option for hourly or daily input data	
OptHyd	-	S	1	N	N	N	Only,OnLine,OffLine,Automatic	Hydrology simulation option	
TimStpHyd	s	S	1	N	N	N	0.001 3600	Calculation time step for hydrology	
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	
OptCalcStabilityWater	-	S	1	N	N	N	Yes,No	Check numerical stability water	
OptCalcStabilitySediment	-	S	1	N	N	N	Yes,No	Check numerical stability sediment	
TimStpWat	s	S	1	N	N	N	0.001 3600	Calculation time step in water layer	If: OptTimStp = Input

ID	Units	Single /Array	Array delimitation	Substance specific	Has distance	Has depth	Limits on value	Description	Comment
TimStpSed	s	S	1	N	N	N	0.001 3600	Calculation time step in sediment	If: OptTimStp = Input
MaxTimStpWat	s	S	1	N	N	N	0.001 3600	Maximum calculation time step in water layer	If: OptTimStp = Calc
MaxTimStpSed	s	S	1	N	N	N	0.001 3600	Maximum calculation time step in sediment	If: OptTimStp = Calc
Section 2									
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	
ConSus	g.m <sup>-3</sup>	S	1	N	N	N	0.0 100000	Concentration of suspended solids	
CntOmSusSol	g.g <sup>-1</sup>	S	1	N	N	N	0.0 1	Mass ratio of organic matter in suspended solids	
AmaMphWatLay	g.m <sup>-2</sup>	S	1	N	N	N	0.0 1000	Dry weight of macrophyte biomass per m2 bottom	
Section 3									

ID	Units	Single / Array	Array delimitation	Substance specific	Has distance	Has depth	Limits on value	Description	Comment
OptFloWat	-	S	1	N	N	N	Transient, Constant	Option for water flow	
OptWaterSystemType	-	S	1	N	N	N	Pond, WaterCourse	Option for selecting the water system type	
OptDis	-	S	1	N	N	N	Fischer, Input	Option for selecting dispersion method	if: OptWaterSystemType = WaterCourse
CofDisPhsInp	m <sup>2</sup> .d <sup>-1</sup>	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 <sup>-1</sup>	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 = Transient and OptWaterSystemType = Pond
QBasPndInp	m <sup>3</sup> .d <sup>-1</sup>	S	1	N	N	N	0.0 50	Base flow, i.e. inflow into pond	if: OptFloWat = Transient and OptWaterSystemType = Pond
HgtCrePnd	m	S	1	N	N	N	0.1 5	Height of the weir crest	if: OptFloWat = Transient and OptWaterSystemType = Pond
WidCrePnd	m	S	1	N	N	N	0.01 10	Width of the weir crest	if: OptFloWat = Transient and OptWaterSystemType = Pond
AreaErsSurPndInp	ha	S	1	N	N	N	0.0 100	Size of the eroding area around the pond	if: OptFloWat = Transient and OptWaterSystemType = Pond and OptLoa = PRZM
AreaUpsWatCrsInp	ha	S	1	N	N	N	0.0 10000	Area of upstream catchment	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
QBasWatCrsInp	m <sup>3</sup> .d <sup>-1</sup>	S	1	N	N	N	0.0 10000	Base flow from upstream catchment	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse

ID	Units	Single / Array	Array delimitation	Substance specific	Has distance	Has depth	Limits on value	Description	Comment
SloBotRepCha	-	S	1	N	N	N	0.0 0.01	Slope bottom representative channel	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
HgtCreRepCha	m	S	1	N	N	N	0.01 5	Height of the weir crest	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
WidCreRepCha	m	S	1	N	N	N	0.01 10	Width of the weir crest	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
LenRepCha	m	S	1	N	N	N	10.0 2000	Length representative channel	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
CofRghRef	s <sup>-1</sup>	S	1	N	N	N	1.0 100	Value Manning coefficient for bottom roughness at 1 m water depth in water body	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
CofVelHea	m.s <sup>-1</sup>	S	1	N	N	N	1.1-1.5	Energy coefficient due to non-uniform distribution of flow velocities in cross section	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
Section 4									
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

ID	Units						Limits on value	Description	Comment
		Single / Array	Array delimitation	Substance specific	Has distance	Has depth			
table horizon SedimentProperties: column 2 Rho	kg.m <sup>-3</sup>	A	no	N	N	N	10 3000	Bulk density	
table horizon SedimentProperties: column 3 CntOm	kg.kg <sup>-1</sup>	A	no	N	N	N	0.0 1	Organic matter mass content	
table horizon SedimentProperties: column 4 ThetaSat	m <sup>3</sup> .m <sup>-3</sup>	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	
FlwWatSpg	m <sup>3</sup> .m <sup>-2</sup> .d <sup>-1</sup>	S	1	N	N	N	0.0 0.01	Rate of percolation through the sediment	
table horizon DispersionLength: column 1 Nr	-	A	no	N	N	N	1 -	Number horizon	Maximally 100 horizons
table horizon DispersionLength: column 2 LenDisSedLiq Section 5	m	A	no	N	N	N	0.01 1	Dispersion length of solute in liquid phase	
MeteoStation	-	S	1	N	N	N	1-25 characters	Name of the *.met file with meteo data	
OptMetInp	-	S	1	N	N	N	Monthly	Option for monthly input data	
Section 6									

ID	Units	Single / Array	Array delimitation	Substance specific	Has distance	Has depth	Limits on value	Description	Comment
Section 7									
table compounds: column 1	-	A	no	Y	N	N	1-15 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 in water	
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 in sediment	
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 <sup>-1</sup>	S	1	Y	N	N	10.0 10000	Molar mass	
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 <sup>-1</sup>	S	1	Y	N	N	-200 200	Molar enthalpy of the vaporization process	

ID	Units	Single /Array	Array delimitation	Substance specific	Has distance	Has depth	Limits on value	Description	Comment
SlbWatRef_[name]	mg.L <sup>-1</sup>	S	1	Y	N	N	0.001 1000000	Water solubility of substance	
TemRefSlb_[name]	C	S	1	Y	N	N	0.0 40	Temperature of reference at which the water solubility was measured	
MolEntSlb_[name]	kJ.mol <sup>-1</sup>	S	1	Y	N	N	-200.0 200.0	Molar enthalpy of the dissolution	
CofDifWatRef_[name]	m <sup>2</sup> .d <sup>-1</sup>	S	1	Y	N	N	0.0 200.0E-5	Reference diffusion coefficient in water	
KomSed_[name]	L.kg <sup>-1</sup>	S	1	Y	N	N	0.0 10000000	Coefficient of equilibrium sorption in sediment	
ConLiqRefSed_[name]	mg.L <sup>-1</sup>	S	1	Y	N	N	0.0 10000000	Reference concentration in liquid phase in sediment	
ExpFreSed_[name]	-	S	1	Y	N	N	0.1 1.5	Freundlich exponent in sediment	
KomSusSol_[name]	L.kg <sup>-1</sup>	S	1	Y	N	N	0.0 10000000	Coefficient of equilibrium sorption suspended solids	
ConLiqRefSusSol_[name]	mg.L <sup>-1</sup>	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 <sup>-1</sup>	S	1	Y	N	N	0.0 10000000	Coefficient for linear sorption on macrophytes	
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	

ID	Units						Limits on value	Description	Comment
		Single /Array	Array delimitation	Substance specific	Has distance	Has depth			
MolEntTraWat_[name]	$\text{kJ.mol}^{-1}$	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]	$\text{kJ.mol}^{-1}$	S	1	Y	N	N	0.0 200	Molar activation enthalpy of transformation	
Section 8									
OptLoa	-	S	1	N	N	N	DriftOnly,PEARL,MACRO,PRZM,GEM	Loading options	
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	$\text{mg.m}^{-2}$	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
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

ID	Units	Single / Array	Array delimitation	Substance specific	Has distance	Has depth	Limits on value	Description	Comment
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 infiltration 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
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
OptUpsInp	-	S	1	N	N	N	Yes,No	Switch for upstream catchment treated	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
RatAreaUpsApp	-	S	1	N	N	N	0.0 1.0	Ratio of upstream catchment treated	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
FraMetForUps_[name]	-	S	1	Y	N	N	0.0 1	Correction factor for primary metabolite formed in water in upstream catchment	if: substance is primary water metabolite and OptFloWat = Transient and OptWaterSystemType = WaterCourse and RatAreaUpsApp > 0
Section 9									
ConSysWatLayIni	g.m <sup>-3</sup>	S	1	N	N	N	0.0 -	Initial total concentration in water layer	
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 <sup>-1</sup>	A	no	N	N	Y	0.0 -	Substance content	maximally 100 values

ID	Units	Single / Array	Array delimitation	Substance specific	Has distance	Has depth	Limits on value	Description	Comment
ConAir	g.m <sup>-3</sup>	S	1	N	N	N	0.0 -	Concentration of the substance in air	
ConWatSpg	g.m <sup>-3</sup>	S	1	N	N	N	0.0 -	Concentration in incoming seepage water	if: FlwWatSpg not zero
Section 10									
OptDelOutFiles	-	S	1	N	N	N	Yes,No	Switch 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	
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
ThiLayTgt	m	S	1	N	N	N	0.00001 1	Thickness of target layer of sediment	
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
OptOutputDepths	-	S	1	N	N	N	None, All, table	Switch output depths	
table OutputDepths: column 1	m	A	no	N	N	Y	0.0 -	Depth	maximally 1000 values

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		maximally every hour in simulation
OptReport	-	S	1	N	N	N	FOCUS	Options for report type	
ExposureReport	-	S	1	N	N	N	Yes,No	Exposure report	
PrintCumulatives	-	S	1	N	N	N	Yes,No	Specify whether fluxes should be cumulated over the entire simulation period	
print_DepWat	m	S	1	N	N	N	Yes,No	Water depth	
print_QBou	m <sup>3</sup> .s <sup>-1</sup>	S	1	N	N	N	Yes,No	Discharge	
print_VelWatFlw	m.d <sup>-1</sup>	S	1	N	N	N	Yes,No	Flow velocity	
print_VolErrWatLay	m <sup>3</sup>	S	1	N	N	N	Yes,No	Volume error in water layer	
print_VvrLiqDra	m.hr <sup>-1</sup>	S	1	N	N	N	Yes,No	Drain flow	if: OptLoa = MACRO
print_FlmDra	g.m <sup>-2</sup> .hr <sup>-1</sup>	S	1	N	N	N	Yes,No	Drain substance flux	if: OptLoa = MACRO
print_VvrLiqRnf	m.hr <sup>-1</sup>	S	1	N	N	N	Yes,No	Runoff (+ infiltration) flow	if: OptLoa = PRZM
print_FlmRnf	g.m <sup>-2</sup> .hr <sup>-1</sup>	S	1	N	N	N	Yes,No	Runoff substance flux	if: OptLoa = PRZM
print_FlmErs	g.m <sup>-2</sup> .hr <sup>-1</sup>	S	1	N	N	N	Yes,No	Erosion substance flux	if: OptLoa = PRZM

ID	Units						Limits on value	Description	Comment
		Single / Array	Array delimitation	Substance specific	Has distance	Has depth			
print_ConLiqWatLay	g.m <sup>-3</sup>	S	1	N	N	N	Yes,No	Concentration in water	
print_CntSorMph	g.kg <sup>-1</sup>	S	1	N	N	N	Yes,No	Content sorbed to macrophytes	
print_CntSorSusSol	g.kg <sup>-1</sup>	S	1	N	N	N	Yes,No	Content sorbed suspended solids	
print_ConSysWatLay	g.m <sup>-3</sup>	S	1	N	N	N	Yes,No	Total concentration in water	
print_ConLiqSed	g.m <sup>-3</sup>	S	1	N	N	N	Yes,No	Concentration in pore water sediment	
print_CntSorSed	g.kg <sup>-1</sup>	S	1	N	N	N	Yes,No	Content sorbed to sediment	
print_ConSysSed	g.m <sup>-3</sup>	S	1	N	N	N	Yes,No	Total content in sediment	
print_CntSedTgt	g.kg <sup>-1</sup>	S	1	N	N	N	Yes,No	Total content in target layer sediment	
print_ConLiqSedTgt	g.m <sup>-3</sup>	S	1	N	N	N	Yes,No	Concentration in pore water in target layer sediment	
print_CntSorSedTgt	g.kg <sup>-1</sup>	S	1	N	N	N	Yes,No	Content sorbed in target layer sediment	
print_MasLiqWatLay	g	S	1	N	N	N	Yes,No	Mass in liquid phase in water layer	
print_MasSorSusSol	g	S	1	N	N	N	Yes,No	Mass sorbed to suspended solids in water layer	
print_MasSorMph	g	S	1	N	N	N	Yes,No	Mass sorbed to macrophytes in water layer	

ID	Units						Limits on value	Description	Comment
		Single / Array	Array delimitation	Substance specific	Has distance	Has depth			
print_MasLiqSed	g	S	1	N	N	N	Yes,No	Mass in liquid phase in sediment	
print_MasSorSed	g	S	1	N	N	N	Yes,No	Mass sorbed in sediment	
print_MasWatLay	g	S	1	N	N	N	Yes,No	Mass in water layer	
print_MasDrfWatLay	g	S	1	N	N	N	Yes,No	Mass entered water layer by spray drift	
print_MasDraWatLay	g	S	1	N	N	N	Yes,No	Mass entered water layer by drainage	
print_MasRnfWatLay	g	S	1	N	N	N	Yes,No	Mass entered water layer by runoff	
print_MasSedInWatLay	g	S	1	N	N	N	Yes,No	Mass penetrated into sediment from water layer	
print_MasSedOutWatLay	g	S	1	N	N	N	Yes,No	Mass transferred from sediment into water layer	
print_MasDwnWatLay	g	S	1	N	N	N	Yes,No	Mass flowed across downstream boundary out of water layer	
print_MasUpsWatLay	g	S	1	N	N	N	Yes,No	Mass flowed across upstream boundary into water layer	
print_MasTraWatLay	g	S	1	N	N	N	Yes,No	Mass transformed in water layer	
print_MasForWatLay	g	S	1	N	N	N	Yes,No	Mass formed in water layer	
print_MasVolWatLay	g	S	1	N	N	N	Yes,No	Mass volatilised in water layer	

ID	Units	Single / Array	Array delimitation	Substance specific	Has distance	Has depth	Limits on value	Description	Comment
print_MasErrWatLay	g	S	1	N	N	N	Yes,No	Mass error in water layer	
print_MasSed	g	S	1	N	N	N	Yes,No	Mass in sediment	
print_MasTraSed	g	S	1	N	N	N	Yes,No	Mass transformed in sediment	
print_MasForSed	g	S	1	N	N	N	Yes,No	Mass formed in sediment	
print_MasWatLayInSed	g	S	1	N	N	N	Yes,No	Mass transferred into water layer from sediment	
print_MasWatLayOutSed	g	S	1	N	N	N	Yes,No	Mass transferred from water layer into sediment	
print_MasDwnSed	g	S	1	N	N	N	Yes,No	Mass leaving sediment across lower boundary	
print_MasErsSed	g	S	1	N	N	N	Yes,No	Mass entering sediment by erosion	
print_MasErrSed	g	S	1	N	N	N	Yes,No	Mass error in sediment	

Note that for most array ID's there is no limit on the length of the array. However in the comment column a maximum number is given. This maximum is what is assigned.

## Annex 3 Technical description of the comprehensive output file

See Annex 2 for legend to table.

ID	Units	Single/Array	Array delimitation	Substance specific	Has distance	Has depth	Limits on value	Description	Comment
Depths of sediment nodes for output in Z-direction column 1	m	A	400	N	N	Y	0 -	Depth in sediment of each node	
Distances of water layer nodes for output in X-direction	m	A	400	N	Y	N	0 10000	Distance in water layer of each node	
Distances of water layer segment interfaces for output in X-direction column 3: Xprofile	m	A	400	N	Y	N	0 10000	Distance in water layer of each interface	number is number of nodes + 1
Xprofile: column 4	-	A	400	Y	N	N	1-15 characters	Substance name	
Xprofile: column 5	m	A	400	N	Y	N	0 10 000	Distance middle of segment from start of water body	
Xprofile: column 6	m	A	400	N	Y	N	0 10	Water depth	
Xprofile: column 7	g.m <sup>-3</sup>	A	400	Y	Y	N	0 -	Total concentration in water	
Xprofile: column 8	g.m <sup>-3</sup>	A	400	Y	Y	N	0 -	Dissolved concentration in water	
column 3: Zprofile									
Zprofile: column 4	-	A	400	Y	N	N	1-15 characters	Substance name	
Zprofile: column 5	-	A	400	N	Y	N	0 400	Segment number from start of water body, where sediment subsystem is located	

ID	Units						Limits on value	Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth			
Zprofile: column 6	m	A	400	N	N	Y	0 -	Depth of middle of segment in sediment	
Zprofile: column 7	m <sup>3</sup> .m <sup>-3</sup>	A	400	N	N	Y	0 1	Porosity	
Zprofile: column 8	g.m <sup>-3</sup>	A	400	Y	N	Y	0 -	Total concentration in sediment	
Zprofile: column 9	g.m <sup>-3</sup>	A	400	Y	N	Y	0 -	Dissolved concentration in sediment	
DepWat	m	A	400	N	Y	N	Yes,No	Water depth	
QBou	m <sup>3</sup> .s <sup>-1</sup>	A	400	N	Y	N	Yes,No	Discharge	
VelWatFlw	m.d <sup>-1</sup>	A	400	N	Y	N	Yes,No	Flow velocity	
VvrLiqDra	m <sup>3</sup> .m <sup>-2</sup> .hr <sup>-1</sup>	A	400	N	Y	N	Yes,No	Drain flow	
VvrLiqRnf	m <sup>3</sup> .m <sup>-2</sup> .hr <sup>-1</sup>	A	400	N	Y	N	Yes,No	Runoff (+ infiltration) flow	
FImDra	g.m <sup>-2</sup> .hr <sup>-1</sup>	A	400	N	Y	N	Yes,No	Drain substance flux	
FImRnf	g.m <sup>-2</sup> .hr <sup>-1</sup>	A	400	N	Y	N	Yes,No	Runoff substance flux	
FImErs	g.m <sup>-2</sup> .hr <sup>-1</sup>	A	400	N	Y	N	Yes,No	Erosion substance flux	
ConLiqWatLay_[name]	g.m <sup>-3</sup>	A	400	Y	Y	N	Yes,No	Concentration in water <sup>15</sup>	
CntSorMph_[name]	g.kg <sup>-1</sup>	A	400	Y	Y	N	Yes,No	Content sorbed to macrophytes	
CntSorSusSol_[name]	g.kg <sup>-1</sup>	A	400	Y	Y	N	Yes,No	Content sorbed suspended solids	
ConSysWatLay_[name]	g.m <sup>-3</sup>	A	400	Y	Y	N	Yes,No	Total concentration in water	
ConLiqSed_[name]	g.m <sup>-3</sup>	A	400	Y	Y	Y	Yes,No	Concentration in pore water sediment	
CntSorSed_[name]	g.kg <sup>-1</sup>	A	400	Y	Y	Y	Yes,No	Content sorbed to sediment	
ConSysSed_[name]	g.m <sup>-3</sup>	A	400	Y	Y	Y	Yes,No	Total content in sediment	
CntSedTgt_[name]	g.kg <sup>-1</sup>	A	400	Y	N	N	Yes,No	Total content in target layer sediment	
ConLiqSedTgt_[name]	g.m <sup>-3</sup>	A	400	Y	N	N	Yes,No	Concentration in pore water in target layer sediment	

<sup>15</sup> The concentration in water, and all other concentrations and contents, is given at the end of the hour. In FOCUS\_TOXSWA 4.4.3 they were given as hour averaged values. In FOCUS\_TOXSWA 5.5.3 these entities were changed, and comply with FOCUS\_TOXSWA 1.1.1 to FOCUS\_TOXSWA 3.3.2.

ID	Units						Limits on value	Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth			
CntSorSedTgt_[name]	g.kg <sup>-1</sup>	A	400	Y	N	N	Yes,No	Content sorbed in target layer sediment	
VolErrWatLay	m <sup>3</sup>	S	1	N	N	N	Yes,No	Volume error in waterbody	
MasWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass in water layer	
MasLiqWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass in liquid phase in water layer	
MasSorSusSol_[name]	g	S	1	Y	N	N	Yes,No	Mass sorbed to suspended solids in water layer	
MasSorMph_[name]	g	S	1	Y	N	N	Yes,No	Mass sorbed to macrophytes in water layer	
MasSed_[name]	g	S	1	Y	N	N	Yes,No	Mass in sediment	
MasLiqSed_[name]	g	S	1	Y	N	N	Yes,No	Mass in liquid phase in sediment	
MasSorSed_[name]	g	S	1	Y	N	N	Yes,No	Mass sorbed in sediment	
MasDrfWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass entered water layer by spray drift	
MasDraWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass entered water layer by drainage	
MasRnfWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass entered water layer by runoff	
MasSedInWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass penetrated into sediment from water layer	
MasSedOutWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass transferred from sediment into water layer	
MasDwnWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass flowed across downstream boundary out of water layer	
MasUpsWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass flowed across upstream boundary into water layer	
MasTraWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass transformed in water layer	
MasForWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass formed in water layer	
MasVolWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass volatilised in water layer	
MasErrWatLay_[name]	g	S	1	Y	N	N	Yes,No	Mass error in water layer	

ID	Units						Limits on value	Description	Comment
		Single/Array	Array delimitation	Substance specific	Has distance	Has depth			
MasTraSed_[name]	g	S	1	Y	N	N	Yes,No	Mass transformed in sediment	
MasForSed_[name]	g	S	1	Y	N	N	Yes,No	Mass formed in sediment	
MasWatLayInSed_[name]	g	S	1	Y	N	N	Yes,No	Mass transferred into water layer from sediment	
MasWatLayOutSed_[name]	g	S	1	Y	N	N	Yes,No	Mass transferred from water layer into sediment	
MasDwnSed_[name]	g	S	1	Y	N	N	Yes,No	Mass leaving sediment across lower boundary	
MasErsSed_[name]	g	S	1	Y	N	N	Yes,No	Mass entering sediment by erosion	
MasErrSed_[name]	g	S	1	Y	N	N	Yes,No	Mass error in sediment	

# Annex 4 The sediment section of the RunId.txw input file for FOCUS\_TOXSWA with recommended layering of the sediment in case of substances with $K_{oc}$ higher than 30 000 L/kg

The values that have to be changed from the standard FOCUS layering are indicated in bold. The sediment layering for substances with high  $K_{oc}$  values consists of 11 layers, whereas the standard FOCUS segmentation consists of 6 layers. In Section 0 Control for the `SedimentTypeID` the `FOCUS_highKoc` sediment is indicated.

```

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

* SedimentProfile table: thickness and number of layers in horizon
* ThiHor Thickness of horizon [0.0001|-]
* NumLay Number of layers in horizon [1|500]
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 ! Sediment properties for ThetaSat and CofDifRel [Input, Calc]

* SedimentProperties table: properties for each horizon:
* Nr Number horizon [1|500]
* Rho Bulk density [10|3000]
* CntOm Organic matter mass content [0|1]
* If OptSedProperties 'Input' then specify ThetaSat and CofDifRel
* ThetaSat Saturated water content [0.001|0.999]
* CofDifRel Relative diffusion coefficient [0|1]
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) ! Percolation rate through the sediment [-0.01|0.01]

* DispersionLength table: dispersion length for each horizon
* Nr Horizon number [1|500]
* LenDisSedLiq Dispersion length of solute in liquid phase (m) [0.01|1]
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

* 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

Parameters that are especially important for the simulation of a water-sediment study have been highlighted.

```
Pond      OptWaterSystemType
No        OptUpsInp

*-----
* Input file for TOXSWA
*
* This file is intended to be used by expert users.
*
* E-mail: toxswa@pesticidemodels.nl
*-----
* (c) Wageningen University & Research
*

* Section 0: Run identification
* Section 1: Control
* Section 2: Waterbody
* Section 3: Hydrology
* Section 4: Sediment
* Section 5: Weather
* Section 6: Temperature
* Section 7: Substance
* Section 8: Loadings
* Section 9: Initial and boundary conditions for mass balance equations
* Section 10: Output control

* This input file considers the current scenario. Input that is not needed for
* this scenario is omitted. For a description of the full input file, see the
* user manual for the FOCUS & ascii version or in your TOXSWA download package.

*-----
* Section 0: Run identification
*
*-----
C3river_Water-sediment  Location          ! Name of the location [1|25 characters]
C3river_WS              WaterbodyID       ! ID of the water body [1|25 characters]
C3river_WS-sediment    SedimentTypeID    ! Name of sediment type [1|25 characters]
WTSD1                   SubstanceName     ! Name of parent substance [1|25 characters]
FOCUS_EXAMPLE           ApplicationScheme ! Name of the application scheme [1|25 characters]

*-----
* Section 1: Control
*
*-----
FOCUS      CallingProgram      ! Release type of scenario [FOCUS]
5.5.3      CallingProgramVersion ! Version numbers for model, interface and database,
           ! respectively
01-Jan-2000 TimStart      ! Start date of simulation [01-Jan-1900 - 31-Dec-9999]
15-Apr-2000 TimEnd        ! End date of simulation [01-Jan-1900 - 31-Dec-9999]

Hourly     OptInp            ! Option for hourly or daily input data of lateral entries [Hourly, Daily]

* OptHyd: options for hydrology simulation
* Only     Simulate only hydrology
* OnLine   Simulate hydrology and substance
* OffLine  Assumption hydrology has been simulated, runID.hyd file must be present
* Automatic TOXSWA checks if hydrology file (runID.hyd) exists; so, hydrology
*          simulation is skipped
OnLine     OptHyd           ! Option selected for hydrology simulation
           ! [Only, OnLine, OffLine, Automatic]

600.       TimStpHyd (s)     ! Calculation time step for hydrology [0.001|3600]

* OptTem: options for temperature simulation
* Only     Simulate only temperature
* OnLine   Simulate temperature and substance
* OffLine  Assumption temperature has been simulated, runID.tem file must be present
* Automatic TOXSWA checks if the temperature file (runID.tem) exists; so, temperature
*          simulation is skipped
OnLine     OptTem           ! Option selected for temperature simulation
           ! [Only, OnLine, OffLine, Automatic, ExtModel]

Input      OptTimStp          ! Time step substance simulation options (Input, Calc)
Yes        OptCalcStabilityWater ! Option for check of stability of the numerical solution for
           ! the water layer
```

```

Yes          OptCalcStabilitySediment ! Option for check of stability of the numerical solution for
          ! the sediment [Yes, No]
          ! Yes = Full check on stability
          ! No = Check on positivity

* If OptTimStp is 'Input' then specify
600.        TimStpWat (s) ! Calculation time step in water layer [0.001|3600]
600.        TimStpSed (s) ! Calculation time step in sediment [0.001|3600]

*-----
*-----
* Section 2: Waterbody
*
*-----

* WaterBody table: description of waterbody
* Len          Length [0.05|]
* NumSeg       Number of segments [1|]
* WidWatSys    Width of the bottom of water system [0.05|100]
* SloSidWatSys Side slope of the water system [0|10]
* DepWatDefPer Water depth defining perimeter for exchange between water layer
*              and sediment [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 [0|100000]
0.           CntOmSusSol (g.g-1) ! Mass ratio of organic matter in suspended solids [0|1]
0.           AmaMphWatLay (g.m-2) ! Dry mass of macrophyte biomass per m2 bottom [0|1000]

*-----
*-----
* Section 3: Hydrology: general
* Section 3a: General
*-----

Constant      OptFloWat          ! Option for water flow (Constant, Transient)

*-----
* Section 3b: Constant water flow
*
* If OptFloWat is 'Constant'
*-----

0.06         DepWat (m)          ! Water depth [0.001|10]
0.           VelWatFlwBas (m.d-1) ! Flow velocity [-1e5|1e5]

*-----
* Section 3c: Variable water flow: pond
*
* If OptFloWat is 'Transient' and OptWaterSystemType is 'Pond'
*-----

*-----
* Section 3d: Variable water flow: watercourse
*
* If OptFloWat is 'Transient' and OptWaterSystemType is 'WaterCourse'
*-----

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

*SedimentProfile table: thickness and number of layers in horizon
* ThiHor      Thickness of horizon [0.0001|-]
* NumLay      Number of layers in horizon [1|500]
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    ! Sediment properties for ThetaSat and CofDifRel [Input, Calc]

* SedimentProperties table: properties for each horizon:
* Nr          Number horizon [1|500]
* Rho        Bulk density [10|3000]
* CntOm      Organic matter mass content [0|1]

```

```

* If OptSedProperties 'Input' then specify ThetaSat and CofDifRel
* ThetaSat Saturated water content [0.001|0.999]
* CofDifRel Relative diffusion coefficient [0|1]
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) ! Percolation rate through the sediment [-0.01|0.01]

* DispersionLength table: dispersion length for each horizon
* Nr      Horizon number [1|500]
* LenDisSedLiq Dispersion length of solute in liquid phase (m) [0.01|1]
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

*-----
*-----

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

C3_river_water_sediment      MeteoStation MeteoStation      ! Name of file with meteo data (*.met)

Monthly      OptMetInp ! Input data [Monthly]

*-----
*-----

* Section 6: Temperature
*
*-----
*-----

* Section 7: Substance
* Section 7a: general
*-----

* Compounds table: first entry is parent, next entries are metabolites [1|15 characters]
table compounds      ! List of substances
WTSD1
end_table

* FraPrtDauWat table: parent-daughter relationships transformation in water
* Column 1: fraction formed from parent into daughter [0|]
* Column 2: name of parent
* Column 3: name of daughter
table FraPrtDauWat (mol.mol-1)
end_table

* FraPrtDauSed table: parent-daughter relationships transformation in sediment
* Column 1: fraction formed from parent into daughter [0|]
* Column 2: name of parent
* Column 3: name of daughter
table FraPrtDauSed (mol.mol-1)
end_table

*-----
* Section 7b: Substance properties for parent WTSD1
* (note extension of parameter name is substance code)
*-----

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

* Volatilization from water layer
1.7E-7      PreVapRef_WTSD1 (Pa)      ! Saturated vapour pressure of substance [0|2e5]
20.      TemRefVap_WTSD1 (C)      ! Reference temperature for saturated vapour pressure
      ! [0|40]
95.      MolEntVap_WTSD1 (kJ.mol-1)      ! Molar enthalpy of vaporization [-200|200]
7.5      SlbWatRef_WTSD1 (mg.L-1)      ! Water solubility of substance [0.001|1e6]
25.      TemRefSlb_WTSD1 (C)      ! Reference temperature for water solubility [0|40]
27.      MolEntSlb_WTSD1 (kJ.mol-1)      ! Molar enthalpy of dissolution [-200|200]

* Diffusion in liquid phase

```

```

4.3E-5      CofDifWatRef_WTSD1 (m2.d-1)      ! Reference diffusion coefficient in water [0|2E-3]

* Sorption
44083.52668 KomSed_WTSD1 (L.kg-1)           ! Freundlich coefficient of equilibrium sorption for
! sediment [0|1e7]
1.          ConLiqRefSed_WTSD1 (mg.L-1)      ! Reference concentration in liquid phase for
! Freundlich coefficient for sediment [0.001|100]
0.9        ExpFreSed_WTSD1 (-)              ! Freundlich exponent in sediment [0.1|1.5]
44083.52668 KomSusSol_WTSD1 (L.kg-1)        ! Freundlich coefficient of equilibrium sorption
! for suspended solids [0|1e7]
1.          ConLiqRefSusSol_WTSD1 (mg.L-1)   ! Reference concentration in liquid phase
! for Freundlich sorption coefficient for
! suspended solids [0.001|100]
0.9        ExpFreSusSol_WTSD1 (-)           ! Freundlich exponent suspended solids [0.1|1.5]
0.          CofSorMph_WTSD1 (L.kg-1)        ! Coefficient for linear sorption on
! macrophytes [0|1e7]

* Transformation in water
0.84       DT50WatRef_WTSD1 (d)              ! Half-life transformation in water at reference
! temperature [0.1|1e5]
20.        TemRefTraWat_WTSD1 (C)           ! Reference temperature for half-life measured in
! water [5|30]
55.        MolEntTraWat_WTSD1 (kJ.mol-1)    ! Molar activation enthalpy of transformation in
! water [0|200]

* Transformation in sediment
590.       DT50SedRef_WTSD1 (d)              ! Half-life transformation in sediment at reference
! temperature [0.1|1e5]
20.        TemRefTraSed_WTSD1 (C)           ! Reference temperature for half-life in sediment
! [5|30]
55.        MolEntTraSed_WTSD1 (kJ.mol-1)    ! Molar activation enthalpy of transformation in
! sediment [0|200]

*-----
* Section 8: Loadings
*-----

* OptLoa options for loading type
* DriftOnly spray drift only entry route
* MACRO      drainage calculated by MACRO
* PRZM       runoff and erosion calculated by PRZM
DriftOnly OptLoa ! Loading option [DriftOnly, PEARL, MACRO, PRZM, GEM]

* Loadings table: details on spray drift, and stretch for all loading types
* Column 1 Date and time of application, relevant if OptLoa is 'DriftOnly', otherwise
* the date is a dummy value
* Column 2 Type of loading [Drift]
* Column 3 Drift deposition (mg.m-2) [0|]
* Column 4 Start of stretch of watercourse loaded by all loading types (m) [0|1e4]
* Column 5 End of stretch of watercourse loaded by all loading types (m) [0|1e4]
table Loadings
end_table

*-----

* Section 9: Initial and boundary conditions for mass balance equations
*-----

* Initial conditions
0.013881 ConSysWatIni (g.m-3) ! Initial total concentration in water layer [0|-]

* CntSysSedIni table: initial total substance content in sediment
* If metabolites are included then initial contents for these substances are set to zero
* Column 1 Depth in sediment (m) [0|-]
* Column 2 Substance content (mg.kg-1) [0|-]
table interpolate CntSysSedIni (mg.kg-1)
end_table

* Boundary conditions
0.          ConAir (g.m-3)                   ! Concentration in air [0|-]
0.          ConWatSpg (g.m-3)                ! Concentration in incoming seepage water [0|-]

*-----

* Section 10: Output control
* Section 10a: General
*-----

No          OptDelOutFiles ! Remove *.out file after simulation [Yes|No]
* DateFormat: options for format of date and time in the output file
* DaysFromSta Print number of days since start of simulation
* DaysFrom1900 Print number of days since 1900
* Years       Print years
DaysFromSta  DateFormat      DateFormat [DaysFromSta, DaysFrom1900, Years]

* RealFormat: format of the ordinary output - use FORTRAN notation:
* e is scientific notation, g is general notation,

```

```

* then the number of positions, then the number of digits
e14.6          RealFormat          ! Format of ordinary output
* OptDelTimPrn: options for output time step
* Hour,Day,Decade,Month,Year Time step for output
* Automatic      Length of simulation period
* Other          User defined
Hour          OptDelTimPrn ! Output time step [Hour|Day|Decade|Month|Year|
                  ! Automatic|Other]

0.025          ThiLayTgt (m)      ! Depth defining the thickness of the target sediment layer
                  ! for output of (averaged) content [1e-5|1]

All          OptOutputDistances ! Options for distances of water layer grid points at which
                  ! output can be obtained[None, All, table]

table        OptOutputDepths    ! Options for depths of sediment grid points at which
                  ! output can be obtained [None, All, table]

* If OptOutputDepths is 'table' then specify
* OutputDepths-table: depths of sediment nodes at which output can be obtained
* Column 1 Depth (m) [0|-]
table OutputDepths (m)
end_table

* Specify dates for output of additional profiles; options set via OptOutputDistances and
* OptOutputDepths are used
* HorVertProfiles table: profiles in horizontal direction for water layer and in vertical
* direction for sediment are given; values given are:
* Water layer: output distance, water depth, total and dissolved concentration,
* Sediment: output node water layer, output depth, pore volume, total and dissolved
* concentration.
table HorVertProfiles
end_table

* Specify type of summary report
FOCUS          OptReport          ! [FOCUS]
Yes            ExposureReport     ! Exposure report [Yes|No]

*-----
* Section 10b: Additional options for Dutch registration report
*
* If OptReport is 'DutchRegistration'
*-----

* Section 10c: Print variables in *.out file
* State variables, fluxes and rates given as momentary values.
* Volume,energy and mass changes given as cumulative values.
*-----

* Specify for all print variables whether output is wanted [Yes, No]
* When print variable is not in file; TOXSWA assumes 'No'

* PrintCumulatives: options for printing cumulatives of volume, energy and mass fluxes
* Yes : cumulative terms have been summed up from start of simulation and have been
*      allocated to the last moment of the period considered
* No  : cumulative terms have been summed up from start of user defined output time step
*      OptDelTimPrn and have been allocated to the last moment of the period
*      considered
No          PrintCumulatives ! [Yes, No]

* Hydrology
No          print_DepWat          ! Water depth (m)
No          print_QBou            ! Discharge (m3.s-1)
No          print_VelWatFlw       ! Flow velocity (m.d-1)
No          print_VolErrWatLay    ! Volume error in waterbody (m3)

* Lateral entries (expressed per m2 adjacent field)

* Concentrations and contents in water layer segments as specified by
* OptOutputDistances
Yes         print_ConLiqWatLay    ! Concentration dissolved in water (g.m-3)
No          print_CntSorMph       ! Content sorbed to macrophytes (g.kg-1)
No          print_CntSorSusSol    ! Content sorbed to suspended solids (g.kg-1)
No          print_ConSysWatLay    ! Total concentration in water (g.m-3)

* Concentrations and contents in sediment below water layer segments as specified by
* OptOutputDistances and OptOutputDepths
No          print_ConLiqSed       ! Concentration in pore water sediment (g.m-3)
No          print_CntSorSed       ! Content sorbed to sediment (g.kg-1)
No          print_ConSysSed       ! Total content in sediment (g.m-3)
Yes         print_CntSedTgt       ! Total content in target layer sediment (g.kg-1)
No          print_ConLiqSedTgt    ! Concentration in pore water in target layer
                  ! sediment (g.m-3)
No          print_CntSorSedTgt    ! Content sorbed in target layer sediment (g.kg-1)

* Distribution in entire water layer
Yes         print_MasLiqWatLay    ! Mass in liquid phase in water layer (g)
Yes         print_MasSorSusSol    ! Mass sorbed to suspended solids in water layer (g)
Yes         print_MasSorMph       ! Mass sorbed to macrophytes in water layer (g)

* Distribution in entire sediment
Yes         print_MasLiqSed       ! Mass in liquid phase in sediment (g)
Yes         print_MasSorSed       ! Mass sorbed in sediment (g)

```

---

```

* Mass balance for entire water layer
Yes      print_MasWatLay      ! Mass in water layer (g)
Yes      print_MasDrfWatLay  ! Mass entered in water layer by spray drift (g)
Yes      print_MasDraWatLay  ! Mass entered in water layer by drainage (g)
Yes      print_MasRnfWatLay  ! Mass entered in water layer by runoff (g)
Yes      print_MasSedInWatLay ! Mass penetrated into sediment from water layer (g)
Yes      print_MasSedOutWatLay ! Mass transferred from sediment into water layer (g)
Yes      print_MasDwnWatLay  ! Mass flowed across downstream boundary out of
! water layer (g)
Yes      print_MasUpsWatLay  ! Mass flowed across upstream boundary into water
! layer (g)
Yes      print_MasTraWatLay  ! Mass transformed in water layer (g)
Yes      print_MasForWatLay  ! Mass formed in water layer (g)
Yes      print_MasVolWatLay  ! Mass volatilised from water layer (g)
No       print_MasErrWatLay  ! Mass error in water layer (g)

* Mass balance sediment
Yes      print_MasSed        ! Mass in sediment (g)
Yes      print_MasTraSed     ! Mass transformed in sediment (g)
Yes      print_MasForSed     ! Mass formed in sediment (g)
Yes      print_MasWatLayInSed ! Mass transferred into water layer from sediment
! layer (g)
Yes      print_MasWatLayOutSed ! Mass transferred from water layer into sediment
! layer (g)
Yes      print_MasDwnSed     ! Mass leaving sediment across lower boundary (g)
Yes      print_MasErsSed     ! Mass entering sediment by erosion (g)
No       print_MasErrSed     ! Mass error in sediment (g)

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

```

---

## Annex 6 Sediment properties of bulk density, porosity and organic matter content; derivation of tortuosity

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:

1. Directly by measurements (e.g. Adriaanse *et al.*, 2014) or
2. By derivation from measurements, e.g. the sediment in the FOCUS surface water scenarios, with its bulk density of 800 kg.m<sup>-3</sup>, 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  $\varepsilon$  (L<sup>3</sup> L<sup>-3</sup>) is the porosity, i.e. volume of liquid divided by volume of sediment,  $\rho_{sed}$  (M L<sup>-3</sup>) is the bulk density of dry sediment, i.e. mass of dry sediment per volume of sediment,  $\rho_{om}$  (M L<sup>-3</sup>) is the phase density of organic matter,  $f_{om, sed}$  (M M<sup>-1</sup>) is the mass fraction of sediment organic matter and  $\rho_{min}$  (M L<sup>-3</sup>) 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  $\rho_{sed}$  and porosity  $\varepsilon$  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<sup>-1</sup> for  $\rho_{om}$  and 2.65 kg L<sup>-1</sup> for  $\rho_{min}$  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<sup>-1</sup> and the standard deviation 0.098 g g<sup>-1</sup> ( $n=19$ ). The large standard deviation suggests that the  $f_{om, sed}$  value is very sensitive to small changes in the  $\rho_{sed}$  and  $\varepsilon$  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, tortuosity can be determined as a function of the porosity, as described below.

The tortuosity factor<sup>16</sup>,  $\lambda$ , 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 A6.1. 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. 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

---

<sup>16</sup> 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.

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 substances, obstructing diffusion.

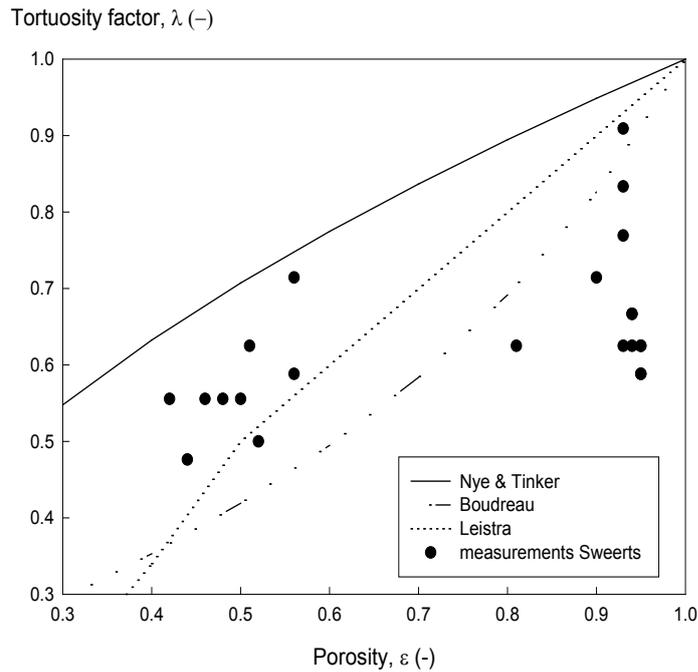


Figure A6.1 The tortuosity factor as function of porosity. The lines indicate tortuosity factors calculated with equations of Nye and Tinker (1977), of Boudreau (1996) and of Leistra (1978). The dots indicate tortuosity factors calculated by Sweerts *et al.* (1991) from measurements in freshwater sediments.

Figure A6.1 shows that at high porosities the tortuosity factors calculated with Boudreau’s equation are closest to Sweert’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  $\rho$  = density, or volumic mass ( $\text{kg m}^{-3}$ ).

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

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

$${}^b\rho_d = \frac{mass\_solid}{bulk\_volume} = \frac{mass\_om + mass\_min}{bulk\_volume} \quad (A3)$$

with  ${}^b\rho_d$ , is the dry bulk density, ( $\text{kg m}^{-3}$ ), 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  $105^\circ\text{C}$  to a constant mass, based on the original volume. The wet bulk density,  ${}^b\rho_w$ , ( $\text{kg m}^{-3}$ ), is defined by

$${}^b\rho_w = \frac{mass\_solid + mass\_liquid}{bulk\_volume} = \frac{mass\_om + mass\_min + mass\_liquid}{bulk\_volume} \quad (A4)$$

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

The organic matter content of sediment is defined as

$$m_{om} = \frac{mass\_om}{mass\_om + mass\_min} \quad (A5)$$

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  $900^\circ\text{C}$ . The solid phase is sieved before entering the oven.

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

$$\varphi = \frac{total\_volume\_of\_pores}{volume\_of\_sediment} \quad (A6)$$

with  $\varphi$  = 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 `ConLiqWatLay_Par` 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), e.g. for the concentration in the 1<sup>st</sup>, 10<sup>th</sup> and 20<sup>th</sup> segment of a stream:

```
3.out 1 4 3 ConLiqWatLay_Par
3.out ! 13 3 ConLiqWatLay_Par
3.out ! 23 3 ConLiqWatLay_Par
```

Gives the following results (only first part of file shown, headers are not given in the file)

```
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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