FOCUS_TOXSWA 5.5.3

Addendum to the manual of FOCUS_TOXSWA 4.4.2

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This document updates parts of the manual of FOCUS_TOXSWA 4.4.2 (Beltman *et al.*, 2014) for FOCUS_TOXSWA 5.5.3.

The updated sections are:

Contents

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

4 User's guide for the TOXSWA user interface

Annexes

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

3.3 Description of the TOXSWA input file

3.3.1 Structure of records in the TOXSWA input file

The TOXSWA input file[1] consists of obligatory and optional records. Each record contains the following fields:

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

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

First, the model scans the entire input file for the record containing the requested identifier. The sequence of records in the file is free. If the requested record is missing, the model either uses default values[2], or prints an error message. If the requested record is found, the model proceeds with verifying the dimension field. This step is followed by the actual data input. Finally, the lower- and upper bounds of the model inputs are checked. In some cases, additional actions are undertaken: model inputs that are specified as a function of 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,
- compound[3] 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:

---

[1] The format of the TOXSWA input file has been changed. However, TOXSWA can still interpret the previous template prepared by FOCUS_TOXSWA 4.4.3. Hence, these input files can still be used with the TOXSWA kernel of FOCUS_TOXSWA 5.5.3.

[2] 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).

[3] 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.

```
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):

```
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 3.3.8). 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
```

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

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

Compound properties
Values have to be supplied for all compounds considered in a simulation run. First, the user

has to specify compound names in the compounds table (see Section 3.3.10). The records are similar to the numerical records, except that to the name of the identifier (field 2) the code of the compound is added (.e.g. _PAR, _MET1 or _MET2 in the example below).

```
100    DT50WatRef_PAR (d)      ! Half-life transformation in water 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 7. 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 7 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	Lay	layer	App	application
Exp	exponent	Area	area	Dis	dispersion	Liq	liquid phase	Avg	average
Fac	factor	Cnt	content	Dra	drainage	Mph	macrophytes	Bal	balance
Fra	fraction	Con	concentration	Drf	drift	Om	organic matter	Bas	base
Mol	molar	Del	difference/delta	Ers	erosion	Sed	sediment	Bot	bottom
Nr	number	Dep	depth	Flo	flow	Sol	solids	Bou	boundary
Num	number	Dst	distance	Flw	flow	Sus	suspended	Cha	channel
Tim	time	DT50	transformation time 50%	For	formation	Sys	water or sediment system	Cmp	compound
		Ent	enthalpy	Hyd	hydrology	Wat	water	Cre	crest
		Flm	mass flux	Inf	infiltration			Crs	course
		Flv	volume flux	Loa	loading			Cum	cumulative
		Fre	Freundlich	Q	discharge			Dau	daughter compound
		Hgt	height	Rnf	runoff			Def	defining
		Kom	om. sorption constant	Sor	sorption			Del	delete
		Len	length	Spg	seepage			Dwn	down to
		Mas	mass	Tor	tortuosity			End	end
		Pre	pressure	Tra	transformation			Err	error
		Rat	rate	Vap	vaporisation			Fld	field
		Rho	bulk density					Hea	energy
		Slb	solubility					Hor	horizon
		Tem	temperature					In	into
		Theta	vol. fraction liquid					Ini	initial
		Thi	thickness					Inp	input
		Vel	velocity					Loc	location

Nature of quantity		Quantity		Process		Phase/domain		Specification	
code	description	code	description	code	description	code	description	code	description
		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	pound
								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 8 gives an overview of the sections in the TOXSWA input file.

Table 8 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 Appendix 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 Fig. 3.2).

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 existent 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

`Only`: The hydrological/temperature module is run, but the remainder

of the simulations is skipped.

```
*-------------------------------------------------------------------------------------------
*-------------------------------------------------------------------------------------------
* 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.

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 ≥ 0`"[4], 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 Fig 3.3).

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

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).

[4] Example of error message, given for waterlayer and RDD not ≥ 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 (itteratively). 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.
```

```
*-------------------------------------------------------------------------------------------------
*-------------------------------------------------------------------------------------------------
* 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.

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

TOXSWA simulates a trapezium-shaped sediment system (see 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.txw` 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^2 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 Fig 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 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 the dispersion is taken into account. The option `OptDis` indicates using an Input value, or calculation the dispersion coefficient according to Fischer (see Appendix 6). When the option Input is selected a value for the dispersion coefficient must be entered `CofDisPhsInp`).

TOXSWA uses only those parameters that concern the selected options in Section 3a for type of water flow and type of waterbody (`OptFloWat, OptWaterSystemType`) in Sections 3b - 3d (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`
3b: Constant flow	x		x	x
3c: Variable flow in a pond		x	x	
3d: Variable flow in a watercourse		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) 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 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.

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.

```
*-------------------------------------------------------------------------------------------------------
*-------------------------------------------------------------------------------------------------------
* 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.

3.3.8 Section 4: Sediment

In this section, the sediment profile, vertical discretization and sediment properties have to be specified (see Fig. 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 segment thickness is taken too large. Furthermore, then mass balance errors may become too large. For most simulations, however, a segment-thickness of 1 to 2 mm in the top 0.01 m, 5 – 10 mm in the 0.01 – 0.05 m sediment layers and 20 and 30 mm for the layers below 0.05 m is a fair compromise.

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

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

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

$$\lambda = \frac{1}{1 - Ln(\varepsilon^2)} \qquad (2)$$

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

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

3.3.9 Section 5: Weather

The Weather section specifies weather data (see Fig 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.

3.3.10 Section 7: Substance properties

The Substance section lists the properties of all compounds (see Fig. 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 compound names (in this example EXSW2). The maximum length of each code is 15 characters.

Section 7a: Compounds and metabolite schemes
A list of compound codes of all compounds in the simulation[5] should be entered in the `table compounds`.

The transformation scheme for compounds formed in water (see also Fig. 3.7) is input in the `table FraPrtDauWat`. For each parent compound, the molar fraction of compound transformed into a daughter must be specified. Figure 3.7 shows an example for three transformations; the parent compound `EXSW2` is for 70% transformed into the daughter `METW1`. This daughter `METW1` is for 100% transformed into a consecutive daughter `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 compounds 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 metabolitesare not shown in Fig. 7).

Section 7b: Substance properties for substance

Molar mass

[5] 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`.

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

Transformation in water
The DegT50 of the compound in the water layer (DT50WatRef) and the temperature at which it is measured (TemRefTraWat) have to be entered. The molar activation enthalpy (MolEntTraWat) adapts the transformation rate in water from the observed temperature to the rate at the temperature of the system (temperatures based on entry from RunId.met file, see Section 3.5).

Transformation in sediment
The DegT50 of the compound 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 3.5).

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

* Compounds table: first entry is parent, next entries are metabolites [1|15 characters]
table compounds
EXSW2
METW1
METW2
METSO
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  METSO -> 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 Compound section in the TOXSWA input file.

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 Fig. 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.txw` 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:

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

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 need to be in this table also.

top layer of the sediment. The eroded soil itself is not accounted for (i.e. the sediment mass is not increased by eroded soil particles).

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 3.3.7) 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 Fig. 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 infiltraton 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 Fig. 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 3.3.8) and the seepage is upward in the water body (negative values) the concentration in incoming seeping 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 tot 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 Fig. 3.10), Section 10b for additional options for Dutch registration report (not described here), and Section 10c to specify which variables are selected to print in the output file (see Fig. 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. Specify the desired (fixed) output interval (`DelTimPrn`). If set to zero, TOXSWA will calculate the output interval based on begin and end date of the simulation. It is important to realize that TOXSWA generates averages over the print interval and not point values. This implies that a larger print interval generates a smoother pattern of resulting values (because calculated values are averaged over a longer period). If `OptDelTimPrn` is `Other`, the time step is set with `DelTimPrn`.

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.

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 segments are given in the output, or if the option All is selected, values for all segments in the sediment are given. If the option `table` is selected, In the `table OutputDepths` can be specified for which depths in sediment output is requested. Then the output for the middle of the segment 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 and segments in sediment for which values are given are set via the options `OptOutputDistances` and `OptOutputDepths`.

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 should include the exposure report (`ExposureReport`).

```
*---------------------------------------------------------------------------------------------
*---------------------------------------------------------------------------------------------
* 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 poinst 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
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.

Section 10b Additional options for 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 those variables of which the output is given as e.g. 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, of since the end of the initialisation period (see the section on `PrintCumulatives` for more details).

```
*-------------------------------------------------------------------------------------------------
* 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 transfered into water layer from sediment
                                ! layer (g)
Yes       print_MasWatLayOutSed ! Mass transfered 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)

3.6 The summary output file

The summary output file has extension .sum (Runld.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 9th line gives the folder on your PC where the simulation was performed. The date on the 110th 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 Runld.sum file differs from the value of the FOCUS drift calculator. Drift calculated with the FOCUS drift calculator is multiplied by 1.2 for stream runs, because of the assumption that 20% of the upstream catchment is treated (FOCUS, 2001). The kind of lateral entry, i.e. drainage or runoff route into surface water is indicated, the soil metabolites that come along, and - only relevant for streams - the correction factor that is used for the fraction metabolite formed in water in the upstream catchment (see Section 4.4.4). The maximum hourly fluxes and the maximum hourly concentrations in drained water or runoff from the entries are given.

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

Mass balances water layer
The mass balance of the substance in the water body is given in tables per month and per year (see Fig. 3.15c). These tables are given for each substance, i.e. the parent and its metabolites. The tables show the numbers with a limited number of decimals for the best readability. Positive values indicate that mass is added, and negative values indicate that mass is reduced.

Mass balances sediment
The mass of the sediment in the whole thickness of the sediment of the entire water body is given in tables per month and per year (see Fig. 3.15d). These tables are given for each substance, i.e. the parent and its metabolites.

```
* ---------------------------------------------------------------------------
* 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       : 30-Nov-2017

* Working directory       : C:\SwashProjects\Project_1\TOXSWA
* Run ID                  : 3
* Input file generated on : 13-12-2017
* ---------------------------------------------------------------------------

* 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.

.

```
*-------------------------------------------------------------------------------
* 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 precipitaton (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 3.15b The summary output file: water balance.

```
* 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
  1978   Nov      0.0000      0.0000      0.1716      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      0.0083     -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      0.0003     -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      0.0001     -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      0.0001     -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      0.0001     -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
  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
  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
  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
  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

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

* ------------------------------------------------------------------------------------------------------------------------------------------------------------------------
* 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
  1978   Nov      0.0031      0.0000      0.0001     -0.0180      0.0211      0.0000     -0.0000      0.0000
  1978   Dec     -0.0019      0.0031      0.0000     -0.0022      0.0004      0.0000     -0.0000      0.0000
  1979   Jan     -0.0003      0.0013      0.0000     -0.0003      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
  1979   Mar     -0.0001      0.0008      0.0000     -0.0001      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
  1979   May     -0.0001      0.0006      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
  1979   Jul     -0.0001      0.0005      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
  1979   Sep     -0.0000      0.0004      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.

Exposure concentrations in water

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

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

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

```
* ------------------------------------------------------------------------------
* 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.

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.

```
* 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.

3.7 The comprehensive output file

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 on 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) of the fluxes are given at the interface of the segments n and n+1

(c) for sediment state variables defined at a node, located in the centre of sediment segment:

```
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 segments.

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

```
Time     Date    Identifier    Value
```

Fig. 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 in the 0-5 m, 45-50 m and 95-100 m segment with nodal points situated at 2.5, 47.5, and 97.5 m distance in the watercourse in segment numbers 1, 10 and 20. The 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 0-0.0001 m, and 0.007-0.010 m segment with nodal points situated at 0.0005 and 0.0085 m distance in the sediment in segment 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 is for 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. In the example `ConSysSed_EXSW2` is shown for segments 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 of the water layer segment interfaces (fluxes). For sediment we did not indicate this as all values refer to sediment nodes, because values for fluxes across sediment segment interfaces are not given as output.

```
* --------------------------------------------------------------------------------

* Results from the TOXSWA model  (c) Wageningen University & Research
* FOCUS  TOXSWA version   : 5.5.3
* TOXSWA model version    : 3.3.6
* TOXSWA created on       : 30-Nov-2017

* Working directory       : C:\SwashProjects\Project_1\TOXSWA
* Run ID                  : 3
* Input file generated on : 13-12-2017
* --------------------------------------------------------------------------------

  Depths of sediment nodes for output in Z-direction:    0.500000E-02   0.450000E-01   0.850000E-01
  Distances of water layer nodes for output in X-direction:                 0.250000E+01   0.750000E+01
0.125000E+02   0.175000E+02   0.225000E+02   0.275000E+02   0.325000E+02   0.375000E+02   0.425000E+02
0.475000E+02   0.525000E+02   0.575000E+02   0.625000E+02   0.675000E+02   0.725000E+02   0.775000E+02
0.825000E+02   0.875000E+02   0.925000E+02   0.975000E+02
  Distances of water layer segment interfaces for output in X-direction:     0.000000E+00   0.500000E+01
0.100000E+02   0.150000E+02   0.200000E+02   0.250000E+02   0.300000E+02   0.350000E+02   0.400000E+02
0.450000E+02   0.500000E+02   0.550000E+02   0.600000E+02   0.650000E+02   0.700000E+02   0.750000E+02
0.800000E+02   0.850000E+02   0.900000E+02   0.950000E+02   0.100000E+03
* Option PrintCumulatives was set to false
* Option OptCalcStabilitySediment was set to true
* Option OptCalcStabilityWater was set to true
* 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   0.000000E+00
0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
0.000000E+00   0.000000E+00
* Unit for CntSedTgt is (mg.kg-1)(values at segment nodes)
    0.000  01-Oct-1978-00h00 CntSedTgt_EXSW2    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
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
1. Day number from start of simulation
2. Date and time
3. Xprofile label indicating horizontal profile in water layer
4. Substance name
5. Distance middle of segment from start of water body (m)
6. Water depth (m)
7. Total concentration in water (g m^{-3})

8. Dissolved concentration in water (g m^{-3})

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

Values that are given in the out file are for water layer segments selected via `OptOutputDistances` and for sediment selected via `OptOutputDepths`. See Sections 3.3.13 and 3.7.1. for more details on this selection. In the example output is given for water layer segments 1, 10 and 20 (distances 2.5, 47.5 and 97.5 m) and for sediment segments 1 and 14 (depths 0.0005 and 0.0085 m), under water layer segment 1, 10 and 20 (see Figure 3.17).

```
29.042  30-May-1986-01h00 XProfile_EXSW2   0.025000E+01  0.320000E+00  0.341848E-10  0.902915E-12
29.042  30-May-1986-01h00 XProfile_EXSW2   0.475000E+02  0.320000E+00  0.341848E-10  0.902915E-12
29.042  30-May-1986-01h00 XProfile_EXSW2   0.795000E+02  0.320000E+00  0.341848E-10  0.902915E-12
29.042  30-May-1986-01h00 ZProfile_EXSW2   1  -0.500000E-03  0.680000E+00  0.902158E-09  0.132670E-08
29.042  30-May-1986-01h00 ZProfile_EXSW2   1  -0.850000E-01  0.680000E+00  0.121909E-07  0.179278E-07
29.042  30-May-1986-01h00 ZProfile_EXSW2  10  -0.500000E-03  0.680000E+00  0.902158E-09  0.132670E-08
29.042  30-May-1986-01h00 ZProfile_EXSW2  10  -0.850000E-01  0.680000E+00  0.121909E-07  0.179278E-07
29.042  30-May-1986-01h00 ZProfile_EXSW2  20  -0.500000E-03  0.680000E+00  0.902158E-09  0.132670E-08
29.042  30-May-1986-01h00 ZProfile_EXSW2  20  -0.850000E-01  0.680000E+00  0.121909E-07  0.179278E-07
```

Figure 3.17 The comprehensive output file; an excerpt of the profile output.

4 User's guide for the TOXSWA user interface

4.3.4 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 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 (Fig. 4.3a). By clicking the button CF the *CF* form can be accessed (Fig. 4.3b).

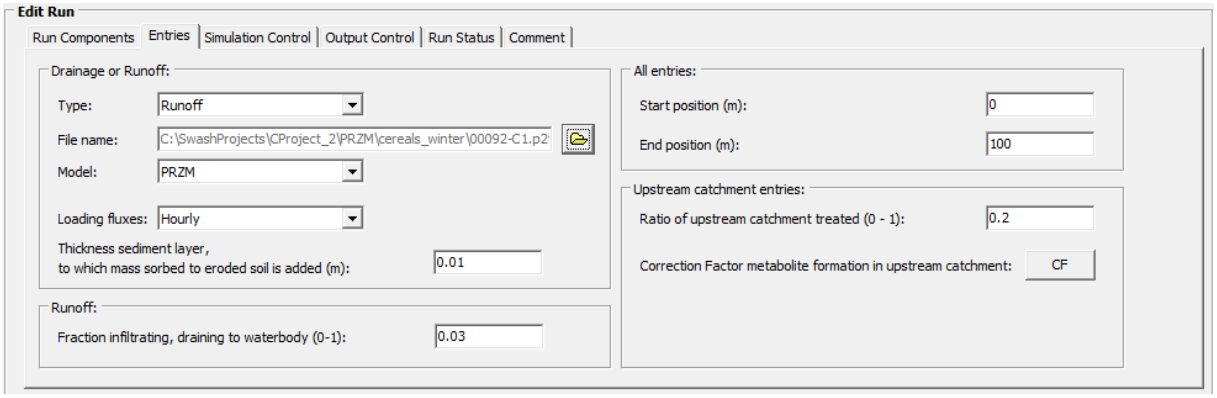

Figure 4.3a Entries tab of the Edit runs form. The section Upstream catchment entries contains the button CF; after clicking on it the correction factors for formation of primary water metabolites in the upstream catchment of FOCUS stream scenarios are shown.

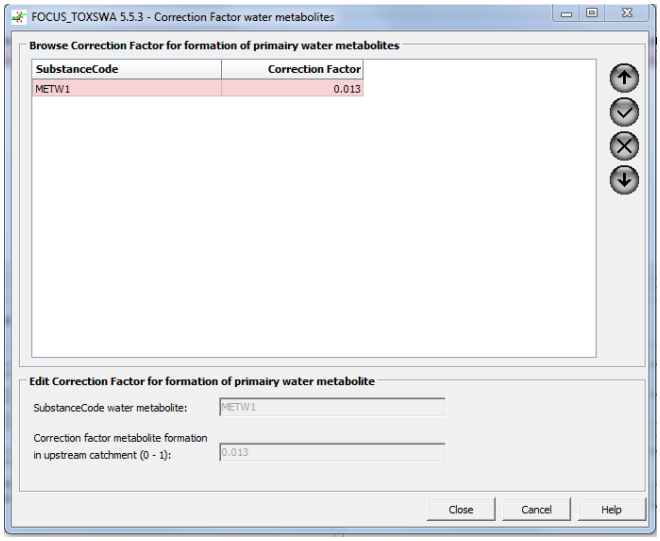

Figure 4.3b Browse Correction Factor water metabolites form.

The correction factor needs to be calculated by the user according to the description given in Appendix 2 of Adriaanse *et al.* (2014). Note that:
a. The factor is only valid for primary metabolites, i.e. metabolites formed directly from the parent,
b. The correction factor is metabolite-specific. c. The correction factor is scenario-specific, because its value is a function of the water temperature and of the residence time in the upstream catchment of the scenario.

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.

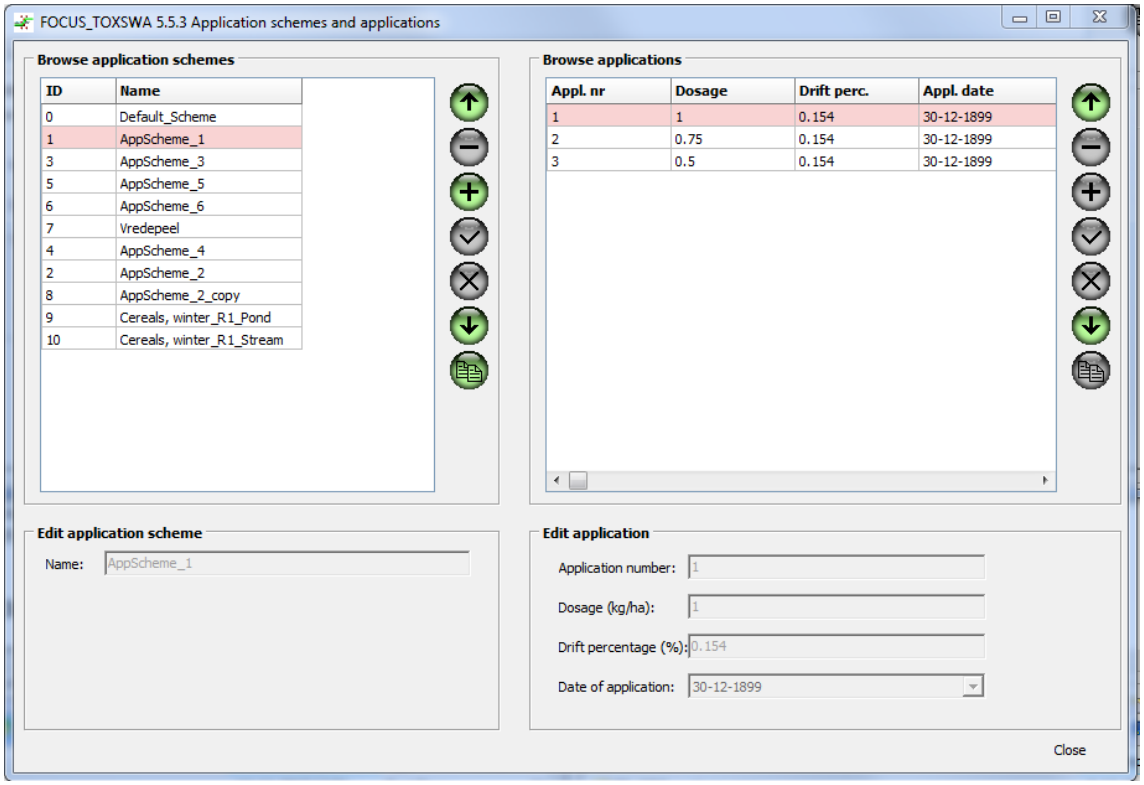

Figure 4.24 The Application schemes and applications form

The drift percentage may be defined by the user or calculated with the FOCUS drift calculator (Appendix H; FOCUS, 2001). The user has to enter the value for the drift percentage manually in the option field, except for FOCUS Step 3 scenarios, where the complete Application 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 ($b + 2 \cdot h \cdot s1$). 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.

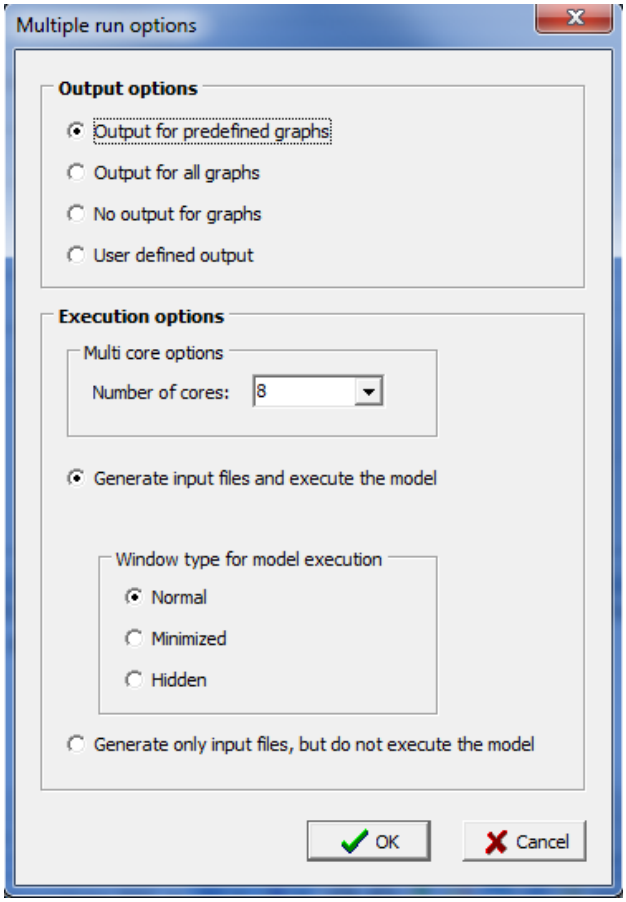

Figure 4.25 Output and execution options offered by TOXSWA when starting a run

Execution options
The calculations can be executed using the multi core 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 4.7.7. When at the Multiple run options form the option 'user defined output' is used, options selected on the Detailed output options forms are used for the simulations (see section 4.12).

Reference

Ter Horst, M.M.S, W.H.J. Beltman, F. Van den Berg, 2016. The TOXSWA model version 3.3 for pesticide behaviour in small surface waters; Description of processes. Statutory Research Task Unit for Nature & the Environment (WOT Natuur & Milieu), WOt-technical report 84. 72p.

Annex 1 FOCUS_TOXSWA input file for expert users

This appendix 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@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

* 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 commentlines 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 nineth
*           position of record (these positions create a clear layout of this txw input file,
*           however,TOXSWA does not discriminate betwwen 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 parametern 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 explictly 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 applicaton 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 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]


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

Weiherbach   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 infiltraton 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 initail contents for these substances are set tot 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 [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 poinst 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 transfered into water layer from sediment
                                ! layer (g)
Yes       print_MasWatLayOutSed ! Mass transfered 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 application scheme	
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-1900I31-Dec-9999	Starting time of simulation	
TimEnd	-	S	1	N	N	N	01-Jan-1900I31-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	0.001I3600	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
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-3	S	1	N	N	N	0.0|100000	Concentration of suspended solids	
CntOmSusSol	g.g-1	S	1	N	N	N	0.0|1	Mass ratio of organic matter in suspended solids	
AmaMphWatLay	g.m-2	S	1	N	N	N	0.0|1000	Dry weight of macrophyte biomass per m2 bottom	
Section 3									

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	m2.d-1	S	1	N	N	N	0.0I1000000	Dispersion coefficient	if: OptWaterSystemType = WaterCourse and OptDis = Input
DepWat	m	S	1	N	N	N	0.001I10	Water depth	if: OptFloWat = Constant
VelWatFlwBas	m.d-1	S	1	N	N	N	-100000.0I100000.0	Flow velocity	if: OptFloWat = Constant
AreaSurPndInp	ha	S	1	N	N	N	0.0I100	Size of area surrounding the pond	if: OptFloWat = Transient and OptWaterSystemType = Pond
QBasPndInp	m3.d-1	S	1	N	N	N	0.0I50	Base flow, i.e. inflow into pond	if: OptFloWat = Transient and OptWaterSystemType = Pond
HgtCrePnd	m	S	1	N	N	N	0.1I5	Height of the weir crest	if: OptFloWat = Transient and OptWaterSystemType = Pond
WidCrePnd	m	S	1	N	N	N	0.01I10	Width of the weir crest	if: OptFloWat = Transient and OptWaterSystemType = Pond

AreaErsSurPndInp	ha	S	1	N	N	N	0.0I100	Size of the eroding area around the pond	if: OptFloWat = Transient and OptWaterSystemType = Pond and OptLoa = PRZM
AreaUpsWatCrsInp	ha	S	1	N	N	N	0.0I10000	Area of upstream catchment	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
QBasWatCrsInp	m3.d-1	S	1	N	N	N	0.0I10000	Base flow from upstream catchment	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
SloBotRepCha	-	S	1	N	N	N	0.0I0.01	Slope bottom representative channel	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
HgtCreRepCha	m	S	1	N	N	N	0.01I5	Height of the weir crest	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
WidCreRepCha	m	S	1	N	N	N	0.01I10	Width of the weir crest	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
LenRepCha	m	S	1	N	N	N	10.0I2000	Length representative channel	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
CofRghRef	s-1	S	1	N	N	N	1.0I100	Value Manning coefficient for bottom roughness at 1 m water depth in water body	if: OptFloWat = Transient and OptWaterSystemType = WaterCourse
CofVelHea	m.s-1	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	0.0001I-	Thickness of horizon	
table Sedimentprofile: column 2 NumLay	-	A	no	N	N	N	1I-	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	1I-	Number horizon	Maximally 100 horizons
table horizon SedimentProperties: column 2 Rho	kg.m-3	A	no	N	N	N	10I3000	Bulk density	
table horizon SedimentProperties: column 3 CntOm	kg.kg-1	A	no	N	N	N	0.0I1	Organic matter mass content	
table horizon SedimentProperties: column 4 ThetaSat	m3.m-3	A	no	N	N	N	0.001I0.999	Saturated water content	
table horizon SedimentProperties: column 5 CofDifRel	-	A	no	N	N	N	0.0I1	Relative diffusion coefficient	
FlwWatSpg	m3.m-2.d-1	S	1	N	N	N	0.0I0.01	Rate of percolation through the sediment	
table horizon DispersionLength: column 1 Nr	-	A	no	N	N	N	1I-	Number horizon	Maximally 100 horizons
table horizon DispersionLength: column 2 LenDisSedLiq	m	A	no	N	N	N	0.01I1	Dispersion length of solute in liquid phase	
Section 5									

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									
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	0.0l-	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	0.0l-	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-1	S	1	Y	N	N	10.0l10000	Molar mass	
PreVapRef_[name]	Pa	S	1	Y	N	N	0.0l200000	Saturated vapour pressure of substance	

TemRefVap_[name]	C	S	1	Y	N	N	0.0I40	Temperature of reference at which the saturated vapour pressure was measured	
MolEntVap_[name]	kJ.mol-1	S	1	Y	N	N	-200I200	Molar enthalpy of the vaporization process	
SlbWatRef_[name]	mg.L-1	S	1	Y	N	N	0.001I1000000	Water solubility of substance	
TemRefSlb_[name]	C	S	1	Y	N	N	0.0I40	Temperature of reference at which the water solubility was measured	
MolEntSlb_[name]	kJ.mol-1	S	1	Y	N	N	-200.0I200.0	Molar enthalpy of the dissolution	
CofDifWatRef_[name]	m2.d-1	S	1	Y	N	N	0.0I200.0E-5	Reference diffusion coefficient in water	
KomSed_[name]	L.kg-1	S	1	Y	N	N	0.0I10000000	Coefficient of equilibrium sorption in sediment	
ConLiqRefSed_[name]	mg.L-1	S	1	Y	N	N	0.0I10000000	Reference concentration in liquid phase in sediment	
ExpFreSed_[name]	-	S	1	Y	N	N	0.1I1.5	Freundlich exponent in sediment	
KomSusSol_[name]	L.kg-1	S	1	Y	N	N	0.0I10000000	Coefficient of equilibrium sorption suspended solids	
ConLiqRefSusSol_[name]	mg.L-1	S	1	Y	N	N	0.001I100	Reference concentration in liquid phase suspended solids	
ExpFreSusSol_[name]	-	S	1	Y	N	N	0.1I1.5	Freundlich exponent suspended solids	
CofSorMph_[name]	L.kg-1	S	1	Y	N	N	0.0I10000000	Coefficient for linear sorption on macrophytes	
DT50WatRef_[name]	d	S	1	Y	N	N	0.1I100000	Half-life transformation in water	

TemRefTraWat_[name]	C	S	1	Y	N	N	5.0I30	Temperature at which half-life was measured	
MolEntTraWat_[name]	kJ.mol-1	S	1	Y	N	N	0.0I200	Molar activation enthalpy of transformation	
DT50SedRef_[name]	d	S	1	Y	N	N	0.1I100000	Half-life transformation in sediment	
TemRefTraSed_[name]	C	S	1	Y	N	N	5.0I30	Temperature at which half-life was measured	
MolEntTraSed_[name]	kJ.mol-1	S	1	Y	N	N	0.0I200	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	mg.m-2	A	no	N	N	N	0.I-	Drift deposition	maximally 1000 values
table Loadings: column 4	m	A	no	N	N	N	0.0I10000	Start of stretch of watercourse loaded by all loading types	maximally 1000 values
table Loadings: column 5	m	A	no	N	N	N	0.0I10000	End of stretch of watercourse loaded by all loading types	maximally 1000 values
WidFldDra	m	S	1	N	N	N	0.0I1000	Width of field contributing drainage	if: OptLoa = MACRO
WidFldRnf	m	S	1	N	N	N	0.0I1000	Width of field contributing runoff	if: OptLoa = PRZM

WidFldErs	m	S	1	N	N	N	0.0|1000	Width of field contributing erosion	if: OptLoa = PRZM
RatInfDir	-	S	1	N	N	N	0.0|1	Ratio of infiltraton water added to runoff water	if: OptLoa = PRZM
ThiLayErs	m	S	1	N	N	N	0.00001|1	Thickness of layer to which erosion mass is added	if: OptLoa = PRZM
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-3	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-1	A	no	N	N	Y	0.0|-	Substance content	maximally 100 values

ConAir	g.m-3	S	1	N	N	N	0.0l-	Concentration of the substance in air	
ConWatSpg	g.m-3	S	1	N	N	N	0.0l-	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 perod	Output time step	If: OptDelTimPrn = Other
ThiLayTgt	m	S	1	N	N	N	0.00001l1	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	0.0l-	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	0.0l-	Depth	maximally 1000 values
table HorizontalProfiles: column 1	-	A	no	N	N	N	StartTimlEndTim		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	m3.s-1	S	1	N	N	N	Yes,No	Discharge	
print_VelWatFlw	m.d-1	S	1	N	N	N	Yes,No	Flow velocity	
print_VolErrWatLay	m3	S	1	N	N	N	Yes,No	Volume error in waterlayer	
print_VvrLiqDra	m.hr-1	S	1	N	N	N	Yes,No	Drain flow	if: OptLoa = MACRO
print_FlmDra	g.m-2.hr-1	S	1	N	N	N	Yes,No	Drain substance flux	if: OptLoa = MACRO
print_VvrLiqRnf	m.hr-1	S	1	N	N	N	Yes,No	Runoff (+ infiltration) flow	if: OptLoa = PRZM
print_FlmRnf	g.m-2.hr-1	S	1	N	N	N	Yes,No	Runoff substance flux	if: OptLoa = PRZM
print_FlmErs	g.m-2.hr-1	S	1	N	N	N	Yes,No	Erosion substance flux	if: OptLoa = PRZM
print_ConLiqWatLay	g.m-3	S	1	N	N	N	Yes,No	Concentration in water	
print_CntSorMph	g.kg-1	S	1	N	N	N	Yes,No	Content sorbed to macrophytes	

print_CntSorSusSol	g.kg-1	S	1	N	N	N	Yes,No	Content sorbed suspended solids	
print_ConSysWatLay	g.m-3	S	1	N	N	N	Yes,No	Total concentration in water	
print_ConLiqSed	g.m-3	S	1	N	N	N	Yes,No	Concentration in pore water sediment	
print_CntSorSed	g.kg-1	S	1	N	N	N	Yes,No	Content sorbed to sediment	
print_ConSysSed	g.m-3	S	1	N	N	N	Yes,No	Total content in sediment	
print_CntSedTgt	g.kg-1	S	1	N	N	N	Yes,No	Total content in target layer sediment	
print_ConLiqSedTgt	g.m-3	S	1	N	N	N	Yes,No	Concentation in pore water in target layer sediment	
print_CntSorSedTgt	g.kg-1	S	1	N	N	N	Yes,No	Content sorbed in target layer sediment	
print_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	
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 transfered 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 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	
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	0I-	Depth in sediment of each node	
Distances of water layer nodes for output in X-direction	m	A	400	N	Y	N	0I10000	Distance in water layer of each node	
Distances of water layer segment interfaces for output in X-direction	m	A	400	N	Y	N	0I10000	Distance in water layer of each interface	number is number of nodes + 1
column 3: Xprofile									
Xprofile: column 4	-	A	400	Y	N	N	1-15 characters	Substance name	
Xprofile: column 5	m	A	400	N	Y	N	0I10 000	Distance middle of segment from start of water body	
Xprofile: column 6	m	A	400	N	Y	N	0I10	Water depth	
Xprofile: column 7	g.m-3	A	400	Y	Y	N	0I-	Total concentration in water	
Xprofile: column 8	g.m-3	A	400	Y	Y	N	0I-	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	0I400	Segment number from start of water body, where sediment subsystem is located	
Zprofile: column 6	m	A	400	N	N	Y	0I-	Depth of middle of segment in sediment	
Zprofile: column 7	m3.m-3	A	400	N	N	Y	0I1	Porosity	
Zprofile: column 8	g.m-3	A	400	Y	N	Y	0I-	Total concentration in sediment	
Zprofile: column 9	g.m-3	A	400	Y	N	Y	0I-	Dissolved concentration in sediment	
DepWat	m	A	400	N	Y	N	Yes,No	Water depth	
QBou	m3.s-1	A	400	N	Y	N	Yes,No	Discharge	
VelWatFlw	m.d-1	A	400	N	Y	N	Yes,No	Flow velocity	
VvrLiqDra	m3.m-2.hr-1	A	400	N	Y	N	Yes,No	Drain flow	
VvrLiqRnf	m3.m-2.hr-1	A	400	N	Y	N	Yes,No	Runoff (+ infiltration) flow	
FlmDra	g.m-2.hr-1	A	400	N	Y	N	Yes,No	Drain substance flux	
FlmRnf	g.m-2.hr-1	A	400	N	Y	N	Yes,No	Runoff substance flux	
FlmErs	g.m-2.hr-1	A	400	N	Y	N	Yes,No	Erosion substance flux	
ConLiqWatLay_[name]	g.m-3	A	400	Y	Y	N	Yes,No	Concentration in water	
CntSorMph_[name]	g.kg-1	A	400	Y	Y	N	Yes,No	Content sorbed to macrophytes	
CntSorSusSol_[name]	g.kg-1	A	400	Y	Y	N	Yes,No	Content sorbed suspended solids	
ConSysWatLay_[name]	g.m-3	A	400	Y	Y	N	Yes,No	Total concentration in water	
ConLiqSed_[name]	g.m-3	A	400	Y	Y	Y	Yes,No	Concentration in pore water sediment	
CntSorSed_[name]	g.kg-1	A	400	Y	Y	Y	Yes,No	Content sorbed to sediment	
ConSysSed_[name]	g.m-3	A	400	Y	Y	Y	Yes,No	Total content in sediment	
CntSedTgt_[name]	g.kg-1	A	400	Y	N	N	Yes,No	Total content in target layer sediment	

ConLiqSedTgt_[name]	g.m-3	A	400	Y	N	N	Yes,No	Concentration in pore water in target layer sediment	
CntSorSedTgt_[name]	g.kg-1	A	400	Y	N	N	Yes,No	Content sorbed in target layer sediment	
VolErrWatLay	m3	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	
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 segmentation of the sediment in case of substances with Koc higher than 30 000 L/kg

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