The CASCADE_TOXSWA model for pesticide behaviour in catchments

Concepts and technical implementation

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This research was done as part of the AquaticRisk@Landscape project, a collaborative TKI subsidised project on the aquatic risk assessment of pesticides at the landscape scale

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TOXSWA

This technical report describes the concepts of the CASCADE_TOXSWA model as well as the technical implementation. CASCADE_TOXSWA is the landscape version of the TOXSWA model. TOXSWA is a so-called exposure model that simulates the fate of substances in surface water in single ponds, ditches and streams. The model is used in the authorization procedures for plant protection products in the Netherlands and in the EU. CASCADE refers to its use in simulating substance fate in and between the interconnected watercourses in a (sub-) catchment. The model has been developed to assess the fate of pesticides in an interconnected system of watercourses in a dynamic hydrological situation. CASCADE_TOXSWA can be used as a stand-alone version, but also as part of a landscape scale system model, to assess e.g. the effect of pesticide use on aquatic organisms. This report describes the concepts of CASCADE_TOXSWA with a focus on the functionalities added as compared to the single watercourse model TOXSWA.

In dit rapport worden de concepten van het CASCADE_TOXSWA model beschreven samen met de technische implementatie. CASCADE_TOXSWA is de landschaps-versie van het TOXSWA model. TOXSWA zelf is een zogenaamd blootstellingsmodel dat de lotgevallen van stoffen in oppervlaktewater simuleert voor enkelvoudige waterlopen, i.e. vijvers, sloten en beken. Het model is onderdeel van de toelatingsprocedures voor gewasbeschermingsmiddelen in Nederland en Europa. CASCADE_TOXSWA simuleert de lotgevallen van stoffen in en uitwisseling tussen de individuele waterlopen van een stroomgebied. Het model is ontwikkeld voor dynamische systemen. Het kan worden gebruikt op zichzelf (stand-alone), maar ook als onderdeel van een landschapsmodel waarin bijvoorbeeld de effecten van het gebruik van gewasbeschermingsmiddelen op waterleven worden gesimuleerd. Dit rapport beschrijft de concepten van CASCADE_TOXSWA met een focus op de aanpassingen die zijn gedaan ten opzichte van TOXSWA.

Keywords: TOXSWA, surface water model, catchment, pesticide fate, environmental risk assessment

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Photo cover: Aerial view of Rummen catchment with streams indicated by bleu lines and orchards by green areas

Aerial view: Esri, Maxa, GeoYe, Earthstar Geographics, CNES/Airbus DS, USDA, USGS, AeroGRID, IGN, and the GIS User Community

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Contents

Verification

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name: B. Buddendorf

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Approved team leader responsible for the contents,

name: Bram de Vos

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1 Introduction

This technical report describes the concepts of the CASCADE-TOXSWA model. CASCADE_TOXSWA is the landscape version of the TOXSWA model. TOXSWA is a so-called exposure model that simulates the fate of substances in surface water in single ponds, ditches and streams. The model is used in the authorization procedures for plant protection products in the Netherlands and in the EU and is one of the models supported by WOT. TOXSWA has model quality status A for versions used in the EU (FOCUS_TOXSWA versions). CASCADE refers to its use to simulate substance fate in and between the interconnected watercourses in a (sub-) catchment. The model has been developed and is currently further developed to assess the fate of pesticides in an interconnected system of watercourses in a dynamic hydrological situation.

1.1 History of CASCADE_TOXSWA

The first version of CASCADE_TOXSWA was realised in 2009. This version was parameterised for a typical Dutch agricultural landscape in the north-east of the Netherlands in the Klazinaveen-Zwartemeer region. The area, with a size of approximately 10 km2, is drained by a network of open drainage ditches with bottom widths between 0.5 and 3 m and a total length of 65 km. The modelled water network consisted of 137 watercourses. The hydrology of the surface water in this area was simulated using the SWQN surface water model (Kruijne et al., 2008). This CASCADE_TOXSWA model was also at a later stage coupled to the effect model MASTEP, a population model for effects on aquatic organisms (Focks et al., 2013). This 2009 first version of CASCADE_TOXSWA covers a limited number of processes and entry routes, e.g. it does not simulate exchange with and transport in the sediment.

1.2 Current developments

From 2018 onwards CASCADE_TOXSWA was redeveloped such that it can be used as a standalone model but also within an integrated modular system. Such an integrated system (Landscape model) organises the simulation of the pesticide sources (e.g. drift deposition, drain emission), the fate of the pesticides and also the ecosystem effects in a landscape. The TOXSWA kernel, which is also used in the FOCUS TOXSWA model, is used as the basis for this module. A wrapper was developed that organises the exchange of information between the TOXSWA kernel and the landscape model. This permits that the TOXSWA kernel functionalities can be easily updated by just incorporating a new version into the CASCADE_TOXSWA module. Technical work and design of the module was mainly done as part of the AquaticRisk@Landscape project, a collaborative TKI project on the aquatic risk assessment of pesticides at the landscape scale (Beltman et al., 2019; Beltman et al., 2020; https://www.tkideltatechnologie.nl/project/wenr20-landscape-appraoch-fate-and-effect-assessments).

This technical report describes the concepts of CASCADE_TOXSWA as implemented from 2018 onwards, with a focus on the functionalities added as compared to the single watercourse model TOXSWA. For the fate concepts as implemented in the TOXSWA kernel we refer to Ter Horst et al. (2017) and Adriaanse (1996).

Note further that the TOXSWA kernel in CASCADE_TOXSWA is now a development line of TOXSWA v.3.

1.3　Definitions used

In the context of CASCADE_TOXSWA for watercourses that are part of a larger catchment the term "*reaches*" is used.

CASCADE_TOXSWA is generally part (or module) of a landscape scale integrated system and simulates the entry of pesticide into the connected reaches of a catchment as well as the fate in these reaches. CASCADE_TOXSWA includes the TOXSWA kernel and a wrapper that organises the exchange between the kernel and the integrated system. An interface, part of the integrated system, provides (i) dynamic output data of a hydrological model for an interconnected set of reaches (hence, the hydrology, i.e. water discharge as well as the dynamic water depth is input for CASCADE_TOXSWA) and (ii) output of a spray drift model (hence spray drift deposition on reaches at specific dates is input for CASCADE_TOXSWA). CASCADE_TOXSWA calculates the concentration in the reaches and the transfer of mass between the reaches, which is collected by the wrapper and provided to the interface. The interface feeds back the output of CASCADE_TOXSWA into the integrated system. Then, this output is available for transfer to e.g. effect modules or for data analysis.

In the context of CASCADE_TOXSWA module the kernel is referred to as *TOXSWA*. The wrapper is referred to as CASCADE-manager.

The integrated system that simulates agricultural management, hydrology, fate (spray drift, drainage, runoff and surface water) and effect at the landscape scale is referred to as *landscape model*. For simulation of fate in surface water the landscape model refers to a system that simulates the hydrology and provides the shape of and the connections between the reaches. The landscape model allows also for the further coupling to effect models and for the storage of data. The landscape model is not discussed in this report.

2 Concepts CASCADE_TOXSWA

2.1 Main concepts

The TOXSWA model simulates the behaviour of pesticides in a water body at the edge-of-field scale, i.e. a ditch, pond or stream adjacent to a single, treated field. It calculates concentrations of pesticides and their metabolites in the water layer and in the sediment due to pesticide entry by drift deposition, drain or runoff entry or atmospheric deposition. An overview of the processes simulated in TOXSWA is given in Figure 1.

suspended solids   macrophytes   sediment solid phase

Figure 1   *Overview of substance fate processes that are simulated in the TOXSWA model. The blue part indicated the processes in the water layer and the orange part indicates the processes in the sediment. Mass exchange between the water and the sediment occurs either by diffusion or by advection.*

TOXSWA considers four processes: (i) transport, (ii) transformation, (iii) sorption and (iv) volatilization (Figure 1). In the water layer pesticides are transported by advection and dispersion, while in the sediment diffusion is included as well. Pesticides are transported across the water-sediment interface by advection (upward or downward seepage) and by diffusion. Transformation of the parent substance into metabolites may be due to hydrolysis, photolysis and biodegradation. The transformation rates and volatilization rates are considered to be temperature dependent. Metabolite formation in water and in sediment is simulated and concentrations in water and sediment of the parent as well as the metabolites can be provided as output (see Adriaanse et al. 2014 background information). Sorption

to suspended solids and to sediment is described by the Freundlich isotherm. Sorption to macrophytes is described by a linear sorption isotherm.

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

TOXSWA simulates a single water body as a water layer divided horizontally in segments with underlying sediment divided vertically in segments (see Figure 2). For example, in the current FOCUS scenarios TOXSWA uses segments of 30 m (ponds, 1 segment), 10 m (ditches, 10 segments) and 5 m (streams, 20 segments) to solve the pesticide mass balance describing the concentration in the water layer. The use of segments allows for simulating a concentration profile over the reach. The mass conservation equation for the transport of the substance in each reach is solved using the explicit integration method as described by Adriaanse (1996).
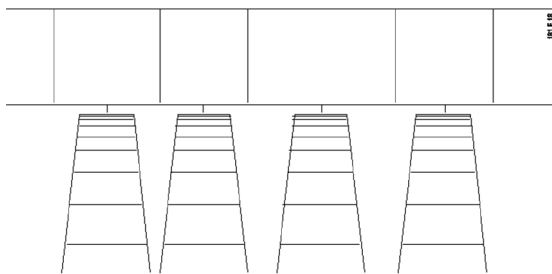

Figure 2   *Transport of pesticides in the pseudo-2D TOXSWA model. Mass balances are solved numerically with the aid of segments in horizontal direction (water layer) and vertical direction (sediment).*

CASCADE_TOXSWA simulates pesticide transport in a catchment with a number of interconnected reaches. Each reach is simulated as a single water body and receives water and mass from upstream reaches. An example of spatial connections is shown in Figure 3. Each reach has its own size and its own numerical segmentation.
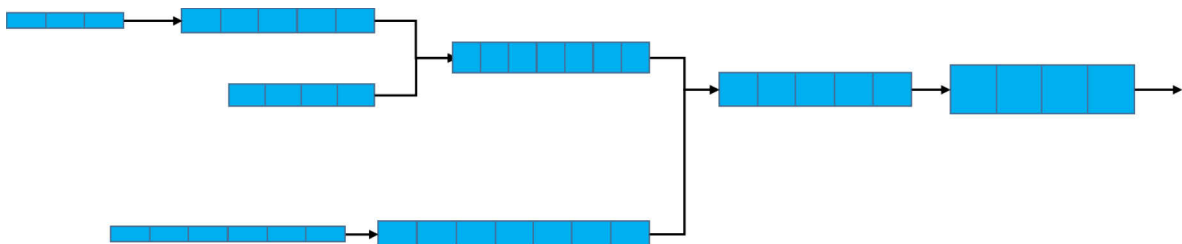

Figure 3   *Transport of pesticides as simulated by the CASCADE_TOXSWA model in a catchment.*

Note that: segmented reaches is under development. In the current version of CASCADE_TOXSWA a reach consists of only one segment.

The CASCADE-manager organises the calling of TOXSWA for simulating the pesticide fate in the individual reaches. It takes care that the simulations start with the most upstream reaches such that downstream reaches receive the input of water and mass from the upstream reaches. The calling of TOXSWA by the CASCADE-manager follows the direction of flow in the catchment, which is assumed to always be towards the outflow (i.e., negative discharges, indicating reversed flow, are not

allowed).When the simulation of the most downward reach is finished the manager extracts and organises the output for all individually reaches. The CASCADE_TOXSWA module can, in turn, be called by a landscape model which organises the simulation of agricultural practices (input), the landscape context, the hydrology etc. Hydrological information is hence provided by an external hydrological model. Flow velocities or discharges for each reach are input for CASCADE_TOXSWA as well as water depth. Initially, all concentrations in water and in sediment are zero.

2.2 Pesticide entry routes

There are four types of lateral input entry[1] of which only spray drift deposition is operational in CASCADE_TOXSWA. For each simulated reach there is also inflow from the upstream reach over the upper boundary.

2.2.1 Spray drift deposition

The spray drift deposition, whose values, timings and location are provided by an external source/program, is simply added to the mass in the reach. Currently, one reach is represented by one segment. All mass that is deposited to a reach is added at the identified date and exact time.

Figure 4 shows an overview on how the spray drift is assigned to the reaches. This assignment is organised by the landscape model, outside CASCADE_TOXSWA. The spray drift is calculated based on a raster projection on the catchment area. This raster projection is translated in a total mass that deposits into a reach (referred to as CASCADE_TOXSWA-1 in Figure 4). In the future CASCADE_TOXSWA will be extended towards more segments per reach. The drift deposition will then be assigned to each individual segment (referred to as CASCADE_TOXSWA-n in Figure 4).
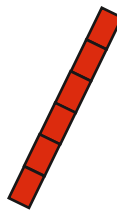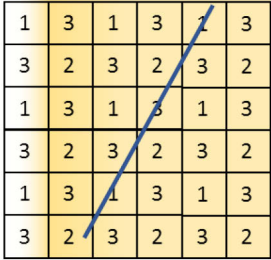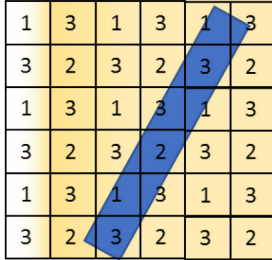

	CASCADE_TOXSWA-1	CASCADE_TOXSWA-n
E-fate reach	hydrology reach	segmented
Spray drift	width water surface not taken into account	width water surface taken into account
	average of cell values crossed by line connecting coordinates, weighed with the length crossed through the cells	average mass per TOXSWA segment, using grid combination of water surface of reach and spray drift deposition cells

Figure 4   *Schematic representation of reach and how grid based spray drift values are derived from output of Xdrift model (Bub et al., 2020).*

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[1]   Drift deposition, drain pipe emission, runoff, atmospheric deposition.

2.2.2 Mass entry at the upper boundary

Water entering at the upper boundary of the reach may contain pesticide mass. The pesticide is transported into the reach. Here only advection is considered:

$$J_{w,ub} = \frac{m_{ub}}{A_{ub}}$$

(1)

with

$J_{w,ub}$ = areic mass flux of substance in water layer by advection at the upstream boundary[2] (kg m^{-2} d^{-1})
m_{ub} = mass flux entering the reach at the upstream boundary of the reach (kg d^{-1})
A_{ub} = wetted cross sectional area of flow at the upstream boundary (m^2)

2.3 Mass flux between reaches

The CASCADE-manager organizes the calling of TOXSWA for simulating the pesticide fate in the individual reaches taking care that the simulations of reaches start with the most upstream reaches. The sequence of calling and the transfer of mass between the reaches is organized by the manager. The simulation of a reach is started after the simulation of the upstream reaches have been finalized. Water discharge and mass flux over the lower boundary of each reach is written down in a csv file and used as input by the downstream reach. The timestep of the downstream mass flux depends on the residence time in a reach, the concepts behind this timestep size derivation are described in this section.

Note that, by simulating the reaches independently only advective transport is simulated between two reaches. The effect of dispersion on the exchange between two reaches is neglected. At the same time numerical dispersion is introduced. Approaches in the scientific literature to include physical dispersion (and hence solve the advection dispersion equation for a system of reaches) are very limited. They require a very high computational effort. Therefore it was decided to only simulate mass transport between reaches due to advection and at the same time allow for numerical dispersion.

The timestep of the water flux depends on and cannot exceed the hydrological timestep in the input file. In principle the timestep can have any size, the current version of CASCADE-TOXSWA has a timestep of 1 hr.

2.3.1 Theoretical considerations on stability

Let us assume a system of interconnected reaches with no sediment layer, only transport and fate processes occur in the water layer and the reaches consist of only one segment. The discharge Q for these reaches is the same at the in- and the outflow of the reach (there is not lateral inflow from drains or runoff). Furthermore, it is assumed that pesticide transport and fate is only due to convection. There are no sources or sinks of pesticide mass (e.g. no degradation). This simplified system is depicted in Figure 5, where *m* is the mass flux [M/T] and *C* is the concentration [M/L^3], *i* is the number of the reach and *i-1* is the upstream reach.

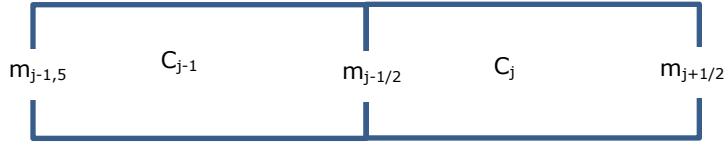[2] (see Eq. (67) in Ter Horst et al., 2017).

Figure 5   *Simplified representation of two reaches with concentrations C and mass fluxes m.*

The mass balance of this system can be written as a first order upwind numerical scheme:

$$\frac{(C)_i^{n+1} - (C)_i^n}{\Delta t} + \frac{m_{i+\frac{1}{2}}^n - m_{i-\frac{1}{2}}^n}{\Delta x} = 0 \tag{2}$$

Where Δt is the timestep [T], n is the timestep number and Δx is the length of a reach [L]. When $m_{i-\frac{1}{2}}^n = uc_i$ and $m_{i+\frac{1}{2}}^n = uc_{i+1}$ we obtain:

$$\frac{(C)_j^{n+1} - (C)_j^n}{\Delta t} + u_j^n \frac{C_j^n - C_{j-1}^n}{\Delta x} = 0 \tag{3}$$

where:
C   = concentration (M/L^3)
u   = Q/A (L/T)
A   = cross-sectional area (L^2)
Q   = discharge (L^3/T)

This is equal to the first order upwind representation of the convection equation, i.e.

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = 0 \tag{4}$$

The local truncation error associated with the tailor series expansion for the convection equation (Eq 3) and this numerical scheme (Eq 3) is then:

$$E_i^n = \frac{1}{2}\Delta t \frac{\partial 2C}{\partial t^2} - \frac{1}{2}\Delta x u \frac{\partial 2C}{\partial x^2} + HOT \tag{5}$$

Where HOT are the Higher Order Terms. With $\frac{\partial 2C}{\partial t^2} = v^2 \frac{\partial 2C}{\partial x^2}$ equation (3) can be rewritten as:

$$E_i^n = v \frac{1}{2}(\Delta t u - \Delta x)\frac{\partial 2C}{\partial x^2} + HOT \tag{6}$$

The modified equation is then:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} - u \frac{1}{2}(\Delta t u - \Delta x)\frac{\partial 2C}{\partial x^2} + HOT \tag{7}$$

Hence, the first order upwind form of the convection equation comes with a truncation error which introduces diffusion, this is also referred to as numerical diffusion/ numerical dispersion.

To get a stable solution the diffusion coefficient must be positive. Rewriting of Equation 7 gives the condition:

$$u\frac{\Delta t}{\Delta x} \leq 1 \qquad (8)$$

$u\frac{\Delta t}{\Delta x}$ is also referred to as the courant number. The CASCADE manager uses this criterion for the exchange of mass between reaches with the rationale: if the assumptions above are relaxed and hence additional fate processes are included, the criterion in Eq 8 is still valid.

This timestep may differ per reach. Note further that by using this criterion numerical dispersion (or diffusion) is accepted and more or less quantified, i.e. by the third term of Eq 7. Implementation is elaborated in Section 2.3.2.

2.3.2   CASCADE_TOXSWA implemented timestep mass flux

For pragmatic reasons it was decided to use the hourly exchange as reference and also as the maximum timestep for mass flux and refine the timestep, based on the courant number, when needed. The number of timesteps in one hour should be a whole number.

Hence:

$$\Delta t = \frac{\Delta x}{u} * k \; ; \; \Delta t = \Delta T/n \qquad (9)$$

Where ΔT is the timestep of the externally provided hydrology, which is now 1 hr; n is a positive integer and k gives an indication of the refinement required as compared to the criterion as given in Eq 8 ($k \leq 1$). Δt may change per hour based on the water velocity u. In case water flow velocities change only per 24 hr, Δt will change also per 24 hr.

k is an input parameter in CASCADE_TOXSWA and considers the entire catchment. A minimum of the time step Δt is applied to prevent numerical problems. The technical procedure is explained in Annex 1.

2.4   Water temperature

For the description of the temperature in the reaches, a simple approach has been implemented. The temperature in the reach system (water layer and sediment) is assumed to remain constant during one day. This daily temperature is calculated as the average of the air temperature on the day itself and of the air temperature of the two days before. This approach is described by EFSA (2020) and by Ter Horst et al. (in prep.) in Chapter 3.

2.5   Model output

Each reach three types of water concentrations can be reported as output; the time weighted concentration (averaged over past hour), the momentary (at the hour) and the hourly maximum concentration (maximum calculated within past hour) and collected in a csv file. An example of momentary concentrations in reaches for a strongly adsorbing substance in the Rummen catchment (Belgium) is shown in Figure 6.

In Annex 4 the results of an example run is shown for one reach at the day of drift deposition and the differences between the three types of concentrations are illustrated. The type of concentration may affect the outcomes of the effect models that calculate the effect of pesticide concentration profiles on aquatic species.
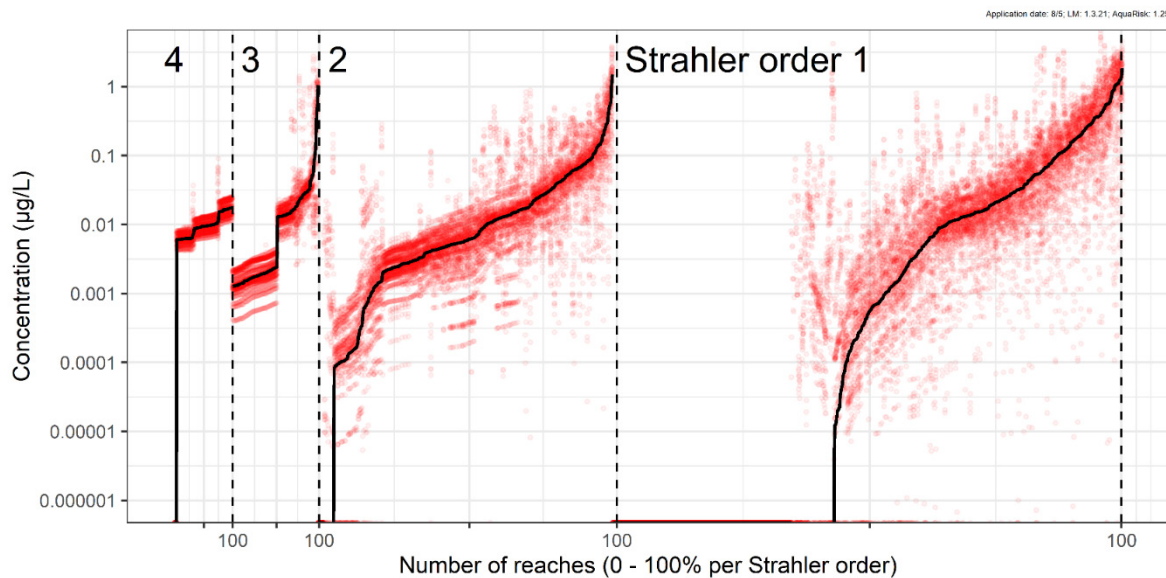
Figure 6   *Example of annual maximum momentary concentrations in reaches of Pyretroid in the Rummen catchment. Maximum concentrations are given for 1735 reaches for 23 years (red circles), given per Strahler order[3] with number of reaches 0 -100%, sorted to the median value of 23 years (black curve). Strahler order 1 are the outermost reaches, hence with smallest discharge (source Beltman et al. 2020).*

A mass balance for the entire catchment can be made from the output. An example is shown for a strongly adsorbing substance applied on fruit orchards in the Rummen catchment in Belgium in Figure 7.

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[3] The stream order or waterbody order is a positive whole number used in geomorphology and hydrology to indicate the level of branching in a river system. According to the "top down" system devised by Strahler, rivers of the first order are the uppermost tributaries. If two streams of the same order merge, the resulting stream is given a number that is one higher. If two rivers with different stream orders merge, the resulting stream is given the higher of the two numbers (Wikipedia, 2021).
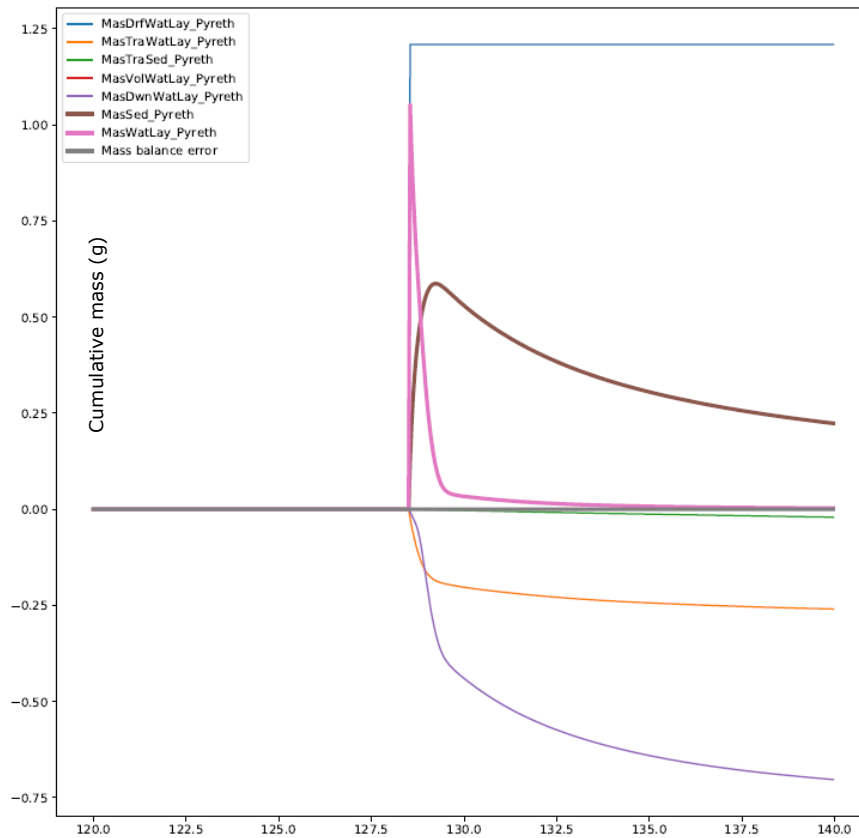
Figure 7   *Example of mass balance output-options for a strongly sorbing substance entering reaches which is applied on day 128 via spray drift in the entire catchment. Mass is given in grams as function of time (plotted per day-of- the-year). (MasDrfWAtLay = total spray drift, MasTraWatLay = total transformed in water layer, MasTraSed = total transformed in sediment, MasVolWatLay = total volatilized, MasDwnWatLay = total flow out of catchment, MasSed = present in sediment, MasWatLay = present in water layer). Negative values indicate loss.*

3 Technical implementation

3.1 General structure

In this chapter the setup of the CASCADE_TOXSWA module and interfaces for the module (= input and output files of module) are described. Figure 8 shows a schematic overview on how the CASCADE_TOXSWA module is structured, and how it connects to the landscape model.
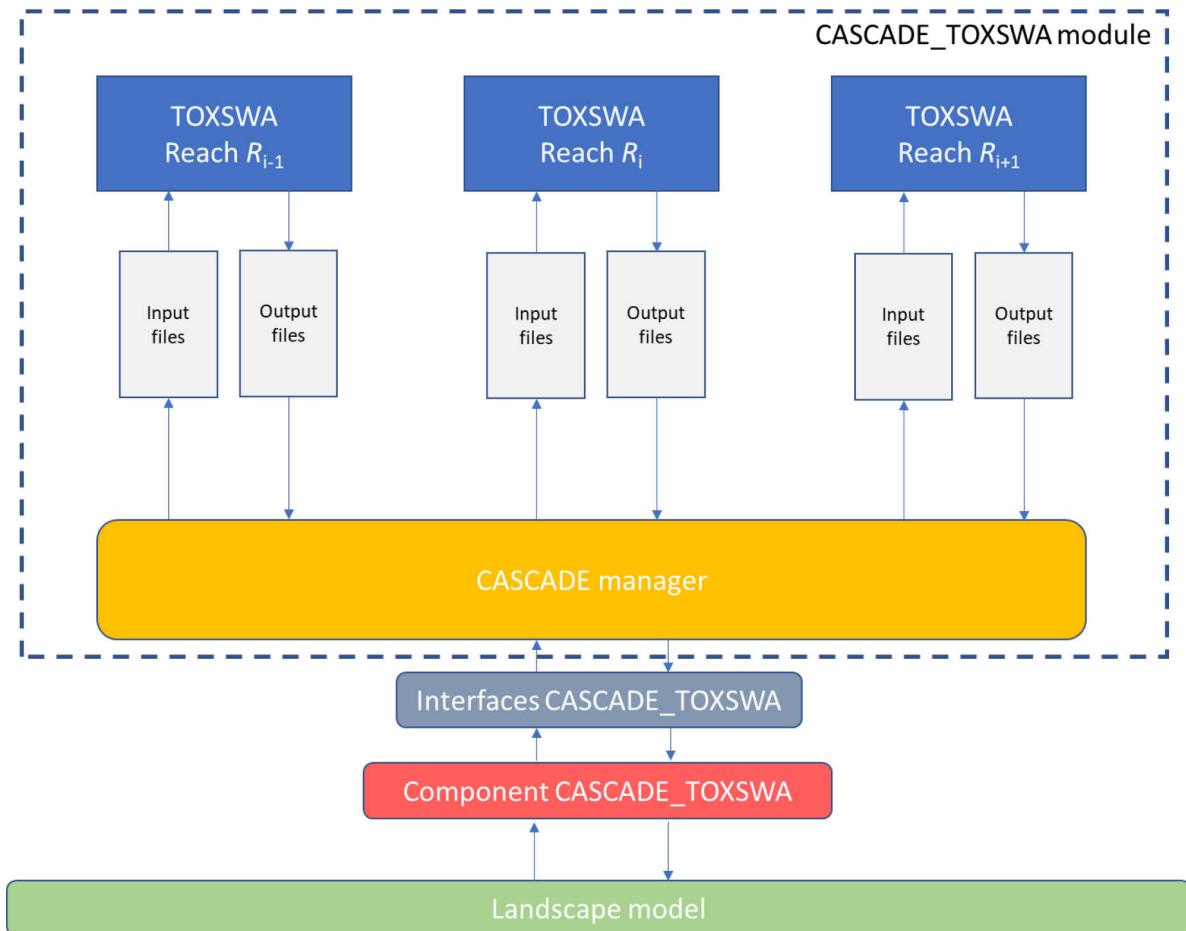

Figure 8   *Schematic of the CASCADE_TOXSWA module, interfaces and component and connections to the landscape model. For each reach a separate TOXSWA run is set up. The CASCADE-manager provides for each run input files that contain: (i) all hydrology related information (ReachID.hyd), (ii) all fate related information (ReachID.twx), (iii) information on the exchange between reaches (ReachID.mfs). These data are provided to the interfaces. The data in the interfaces are written by the component on the basis of data available in the landscape model.*

The CASCADE-managers' main goal is to exchange parameters and states between the landscape model (via CASCADE_TOXSWA interfaces and component) and TOXSWA and to initiate and end the calling of the TOXSWA runs.

The interface specifies how the data has to be provided to CASCADE_TOXSWA (format, semantics) and which output should be provided by CASCADE_TOXSWA. The "physical" representation of this interface, i.e. all the inputs and outputs, is given in section 3.3.

The CASCADE_TOXSWA component implements the same interface, however, with inverted roles. That is, the component writes data that can be read by CASCADE_TOXSWA, and reads data that is written by CASCADE_TOXSWA, both thanks to an agreed interface. The component implements a second interface (the "Landscape Model API") that allows to exchange data with the Landscape Model core. In essence, the component functions as a translator between the Landscape Model core and CASCADE_TOXSWA.

The component, interfaces and module are together one software package that simulates fate of pesticides with TOXSWA at the landscape scale.

The landscape model starts the CASCADE_TOXSWA module and provides the required information regarding (spatially distributed) environmental characteristics and drift deposition mass and geolocation as well as the required reach dimensions and connections. The CASCADE-manager reads the data from the interfaces to prepare the input for the TOXSWA runs. After finalization of the calculations the CASCADE-manager provides the output to interfaces. The component transfers the data back into the landscape model. The data feed back into the Landscape model and can be made available to effect modules or used for data processing or graphical output.

In this chapter we only describe the additional functionalities as compared to the TOXSWA kernel. We refer to e.g. ter Horst et al. (2017) for details on the processes implemented in TOXSWA. The input and output of TOXSWA is described in Beltman et al. (2018). The additional input and output for use in CASCADE_TOXSWA is described in Annex 1 and concerns mainly the connection between reaches, which is needed for mass exchange between reaches. Hence the description in this chapter mainly concerns the implementation of the CASCADE-manager and the interfaces. In the final section, section 3.8, some remarks about the TOXSWA kernel are given, relevant for using the TOXSWA kernel in the CASCADE_TOXSWA context.

3.2 CASCADE-manager procedures

3.2.1 Introduction

The main tasks carried out by the CASCADE-manager are:
- Preparing/copying the necessary TOXSWA input files for each reach
- Running the TOXSWA simulations for the reaches
- Extracting variables and from the TOXSWA output files converting them to CSV format

These are described in more detail in sections 3.3.2 to 3.3.4.

3.2.2 Initialization and creation of TOXSWA input files

The initialization tasks of the CASCADE-manager are:
- Preparing the hydrology file for each reach, the ReachID.hyd containing hourly values of discharge and water depth.
- Preparing the ReachID.txw file; including the spray drift entries table for the whole simulation period, the reachID's of the reaches upstream and of the reach downstream of the reach, the value for the depth defining perimeter (see explanation box below).
- This depth defining perimeter is set to the lowest water depth of the simulation period (derived from the hydrological data)
- Deriving the time step for exchange of mass flux between reaches for each reach based on the flow velocity of the downstream reach for each hour, and writes these time steps to the ReachID.mfs file. (see Annex 1 for more detail)

Definition depth defining perimeter

The depth defining perimeter is the height of side slope of the reach taking part in exchange of mass between water and sediment is the minimum water depth occurring in the simulation (see Figure 9; section 4.2.1 in ter Horst et al., 2017)
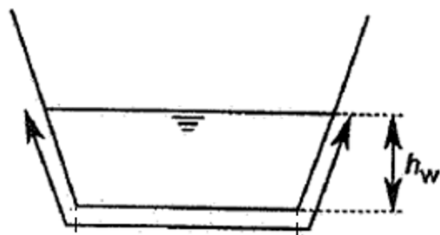

Figure 9   *Cross section of the reach; the depth defining perimeter h_w defines up to which part of the sediment layer substance is exchanged between water and sediment; h_w should be equal to or below the lowest water level occurring in the simulation period.*

TOXSWA runs and writes at the end of each simulated hour the concentration in the reach and the mass flux to the next (downstream) reach in the file (ReachID.mfu). The TOXSWA runs are finalized on the end time given in the txw file.

The TOXSWA input file provides all input information for each run. One standard template input file is used for CASCADE_TOXSWA in which reach and catchment specific information is added. In Annex 3 this template is provided. In Annex 2 the main characteristics of the TOXSWA parameterisation is given.

3.2.3   Running TOXSWA simulations

During the simulation the CASCADE-manager distributes the runs over the processors and control the runs.

It is possible that a reach does not receive any substance over the simulation period, i.e. neither the reach itself nor any of the reaches in the upstream part of the catchment receive drift input. In this case, the simulation isnot done and the downstream reach is informed that the output concentration is zero over the simulation period. Moreover, simulation is also skipped if for a reach pre-existing output files from a previous run are present in the working directory.

When the simulation of a reach stops because the numerical solution for the sediment cannot be solved, the value for the maximum time step in sediment is devided by two replacing the value that was set in the ReachID.txw file. This procedure is repeated until the reach is simulated successfully.

Currently, a simulation of a reach can only start if the simulation for all of its upstream reaches is finished. The scheduling of the simulations is handled using a dynamic scheduler which keeps track of the reaches for which the simulation can start.

The scheduler allows for running multiple simulations simultaneously while using different processors for reaches between which no dependency exists. It should be noted that the number of simulations that can be run in parallel depends on the topology of the catchment and will generally decrease when moving downstream in the catchment. A run for a reach is started only when results of upstream reaches are available.

3.2.4   Finalization and extracting TOXSWA output

After the simulation is finished for a reach, the output variables are extracted by the CASCADE-manager from the TOXSWA output files and converted to a CSV file named ReachID.csv. For skipped reaches a dummy output file containing only zeros, is created. Generating a mass balance for the whole catchment is optional. Hence, finalization steps are:

- Writing a csv file for each reach ReachID.csv with hourly values of selected output variables, e.g. concentration and mass in water layer. This csv file is a CASCADE_TOXSWA interface (see Figure 8) and is written after finalization of the run and can via the CASCADE_TOXSWA module (see Figure 8) further distribute these concentrations to the effect modules.
- Calculating the mass balance of the catchment using the output of the individual TOXSWA runs and write it to a file for the full catchment (this is an option, and is not standard when running the landscape model).

3.3 Interfaces: input files for CASCADE_TOXSWA

The following input files (these are the CASCADE_TOXSWA interfaces) are required and need to be made prepared by the CASCADE_TOXSWA module of the landscape model (see Figure 8):
- Configuration file: specifies the simulation configuration, and other input files (e.g. config.ini)
- Reach specification file: contains data concerning reach & reach network (e.g. Reaches.csv)
- Hydrology and mass loadings file: contains hydrology and mass loadings for every hour of the simulation. Needed for each reach which should be simulated (e.g. ReachID.hyd)
- Temperatures file, containing daily temperatures for the whole catchment (e.g. temperature.csv)
- Substances file: contains substance properties for the parent and the metabolites (e.g. substances.csv)

3.3.1 Configuration file

The simulation configuration is specified in the configuration file, the name of which is passed to the CASCADE-manager as command line argument. This file is structured according to the "Windows ini" format. It is subdivided into sections, which are denoted by square brackets (e.g. [section1]). Each section specifies configuration parameters in format: key=value. The order of the parameters is not relevant, but parameters must be located in the correct section. Table 1 lists the required attributes.

3.3.2 Reach specification file

For a catchment there is one reach specification file, specified in the configuration file (parameter reachFile). It must be located in the input directory specified in the configuration file (parameter inputDir). This file lists for every reach its ID, its downstream reaches, and properties needed by TOXSWA. It should be structured as comma separated values. The first two rows contain the column headers and the units for the attributes. The following rows specify for every reach all attribute values. Table 2 lists all the attributes.

Example reach specification file

```
RchID,RchIDDwn,Len,WidWatSys,SloSidWatSys,ConSus,CntOmSusSol,Rho,ThetaSat,CntOM,X,Y,Expsd

-,-,m,m,-,g/m3,g/g,kg/m3,m3/m3,g/g,-,-,-

R680,678,100.0,0.3,5.0,1.0,0.09,800,0.6,0.09,210607.26712649316,162595.8278469257,False

R681,680,100.0,0.3,5.0,1.0,0.09,800,0.6,0.09,210666.67049544305,162515.38486965373,False
```

Table 1 *Required attributes of the configuration file of CASCADE_TOXSWA.*

Key	Description	Format	Example	Comment
Section [general]				
nWorker	Number of workers	integer	1	1: serial run; >1: parallel run
inputDir	Directory containing input specific to this run	Directory path	input	Can be an absolute path or relative to the root module directory
experimentName	Name for simulation experiment	String	Experiment_1	Should be usable for path names (so no forbidden characters in name)
reachSelection	List of reaches for which to run	Comma-separated list of reach IDs, or "all"	• all • R1, R2, R3	If "all" is specified, all reaches found in the reachFile will be simulated
reachFile	Name of file specifying reach properties	Filename	Reaches.csv	This file should be located in inputDir
startDateSim	Start date of the simulation	Date in format "DD-MM-YYYY"	01-Jan-1992	
endDateSim	End date of the simulation	Date in format "DD-MM-YYYY"	31-Dec-1992	
Section [toxswa]				
toxswaDir	Directory containing TOXSWA executable and other necessary files	Directory path	TOXSWA	Can be an absolute path or relative to the root module directory
timeStepDefault	Default time step length (s)	Float	600	
timeStepMin	Minimum time step length (s)	Float	100	
temperatureFile	Name of temperature file	Filename	Temperature.csv	This file should be located in inputDir
substanceFile	Name of substance file	Filename	substance.csv	This file should be located in inputDir
substanceNames	Name of the substance for which to simulate	String	SubstanceA	Currently only one substance is supported
timeStepMin	Minimum time step length	float	100	
outputVars	List of output variables which should be output by TOXSWA	Comma-separated list	ConLiqWatTgtAvg, ConLiqWatTgtAvgHrAvg and ConLiqWatTgtAvgHrMax, MasWatLay	
keepOrigOutFiles	Switch indicating whether or not to keep the original TOXSWA output files (.out) in the working directory	[True	False]	False	
massFlowTimestepParam	Parameter k controlling the time step of mass flux exchange between reaches	Float	1	
minMassFlowTimestep	Minimum time step of mass flux exchange between reaches, supersedes effect of massFlowTimestepParam on the timestep, Δt, if $\Delta t < minMassFlowTimeStep$	Float	0.1	Optional, default = 1
deleteMfuFiles	Switch specifying whether MFU files containing mass fluxes between reaches should be deleted when they are no longer needed	[True	False]	True	Optional, default = False.

Table 2 *Attributes of the reach specification file.*

Variable	Units	Format	Column header
Reach ID	n/a	arbitrary	RchID
Downstream reach IDs	n/a	Comma-separated list in double quotes	RchIDDwn
Length	m	Standard, prec. 0.1 m	Len
Width bottom of reach	m	Standard, prec. 0.01 m	WidWatSys
Slope of bank of reach (dx/dz)	-	Standard, prec. 0.01	SloSidWatSys
Suspended solids	g/m3	Standard, prec. 0.1 g	ConSus
Organic matter content suspended solids*	g/g	Standard, prec. 0.01 g/g	CntOmSusSol
Bulk density sediment	kg/m3	Standard, prec. 1 kg/m3	Rho
Porosity sediment	m3/m3	Standard, prec. 0.01 m3/m3	ThetaSat
Organic matter content sediment*	g/g	Standard, prec. 0.01 g/g	CntOM
x-coordinate middle of reach	-	Standard, prec. 0.0001	X
y-coordinate middle of reach	-	Standard, prec. 0.0001	Y
Spray drift entry during simulation period	-	TRUE/FALSE	Expsd

*Organic matter content can be calculated from OC content by multiplication with a factor 1.742.

3.3.3 Hydrology and mass loadings files

For each reach to be simulated a file named ReachID.csv is prepared (see Figure 8). ReachID is the reach ID, specified in the reach specification file. The files should be located in the input directory specified in the configuration file (inputDir). The files should be structured along comma separated values. The first two rows contain the column headers for the attributes, and the units. The following rows specify for every time step all attribute values. Table 3 lists all the attributes.

Example hydrology and mass loadings file

```
Time,QBou,DepWat,LoaDrf
-,m3.s-1,m,mg.m-2
07-May-2007-01h00,2.794203E-05,0.419,0.000000E+00
07-May-2007-02h00,2.738870E-05,0.415,0.000000E+00
```

Table 3 *Attributes of the hydrology and mass loadings file.*

Variable	Units	Format	Column header
Date-time	arbitrary	arbitrary	Time
Water discharge	$m^3 s^{-1}$	scientific, ≥4 sig. digits	QBou
Water depth	m	Standard, prec. 0.001 m	DepWat
Mass loading spray drift*	mg m^{-2}	scientific, ≥4 sig. digits	LoaDrf

*Unit is mg per m^2 of water surface.

3.3.4 Temperature file

There is a single file for all reaches, listing for every reach its ReachID, its downstream reaches, and properties needed by TOXSWA. The name of this file is specified in the configuration file. The file should be structured as follows, and uses comma separated values. The first two rows contain the column headers for the attributes, and the units. The following rows specify for every reach all attribute values. Table 4 lists all the attributes.

Table 4   *Attributes of the hydrology and mass loadings file.*

Variable	Units	Format	Column header
Date	arbitrary	arbitrary	Time
Average daily air temperature*	C or K	Standard, prec. 0.01 C/K	TemAir

*If hourly data are available then the daily average temperature should be calculated from these hourly values. However if only maximum and minimum daily temperature are available, these two values can be averaged.

Example temperature file

```
Time,TemAir

-,C

01-Oct-1978,4.01

02-Oct-1978,4.53
```

3.3.5   Substance file

There is one file containing substance parameters. The name of this file is specified in the configuration file. The first row is the parent substance name. Next lines are metabolites (the use of metabolites is not yet implemented for the CASCADE-manager). Table 5 lists all the attributes. Default values for parameters are given as well (conform FOCUS Surface Water).

Table 5 *Attributes of the Substance file.*

Variable	Units	Default value	Format	Column header
Substance name	-	-	max. 15 characters	SubName
Molar mass	g.mol^{-1}	-	standard, prec. 0.1 g/mol	MolMas
Saturated vapour pressure	Pa	-	scientific, ≥2 sig. digits	PreVapRef
Reference temperature for saturated vapour pressure	°C	20	standard, prec. 0.1 °C	TemRefVap
Molar enthalpy of vaporization	kJ/mol	95	standard, prec. 1 kJ/mol	MolEntVap
Solubility in water	mg/L		standard, prec. 0.1 mg/L	SlbWatRef
Reference temperature for water solubility	°C	20	standard, prec. 0.1 °C	TemRefSlb
Molar enthalpy of dissolution	kJ/mol	27	standard, prec. 1 kJ/mol	MolEntSlb
diffusion coefficient	m^2.d^{-1}	4.3.10^{-5}		CofDifWatRef
Reference temperature for diffusion	°C	20	standard, prec. 0.1 °C	TemRefDif
Half-life transformation in water	d	-	standard, prec. 0.1 d	DT50WatRef
Temperature at which half-life in water was measured	°C	20	standard, prec. 0.1 °C	TemRefTraWat
Molar activation enthalpy of transformation in water	kJ/mol	65.4	standard, prec. 0.1 kJ/mol	MolEntTraWat
Half-life transformation in sediment	d	1000	standard, prec. 0.1 d	DT50SedRef
Temperature at which half-life in sediment was measured	°C	20	standard, prec. 0.1 °C	TemRefTraSed
Molar activation enthalpy of transformation in sediment	kJ/mol	65.4	standard, prec. 0.1 kJ/mol	MolEntTraSed
Coefficient for equilibrium sorption in sediment	L/kg	-	standard, prec. 0.1 L/kg	KomSed
Reference concentration in liquid phase in sediment	mg/L	1	standard, prec. 0.1 mg/L	ConLiqRefSed
Freundlich exponent in sediment	-	0.9	standard, prec. 0.01	ExpFreSed
Coefficient for equilibrium sorption of suspended solids	L/kg	-	standard, prec. 0.1 L/kg	KomSusSol
Reference concentration for suspended solids	mg/L	1	standard, prec. 0.1 mg/L	ConLiqRefSusSol
Freundlich exponent for suspended solids	-	0.9	standard, prec. 0.01	ExpFreSusSol
Coefficient for linear sorption on macrophytes	L/kg	0	standard, prec. 0.1 L/kg	CofSorMph
Number of metabolites formed in water	-	0	integer	NumDauWat
Substance name**	-	-	max. 15 characters	SubName***
Fraction formed from parent into daughter***	mol/mol	-	standard, prec. 0.01	FraPrtDauWat
Number of metabolites formed in sediment	-	0	integer	NumDauSed
Substance name****	-	-	max. 15 characters	SubName***
Fraction formed from parent into daughter****	mol/mol	-	standard, prec. 0.01	FraPrtDauSed

* Organic matter content can be calculated from OC content by multiplication with a factor 1.742.

** If there are metabolites NumDauWat > 0; then NumDauWat substance names and their fraction formed from parent must be given.

*** For this substance all properties must be entered in a row in the table.

**** If there are metabolites NumDauSed > 0; then NumDauSed substance names and their fraction formed from parent must be given.

3.3.6   Template of input file for TOXSWA kernel

In Annex 3 the template of the TOXSWA input file (ReachID.txw) is given.

3.4   Output files of CASCADE_TOXSWA

The CASCADE-manager produces one output file for every reach, named ReachID.csv, containing model results. Which outputs[4] are requested is indicated in the configuration file of the CASCADE-manager.

The name of the ReachIDs is given in the reach specification file. In the column headers the variable names are suffixed by the substance name (specified in the configuration file), separated by an underscore. Table 6 specifies the columns and variables. XXXX in the column-header corresponds to Substance_name in the Substances.csv file. Except for the variables ConLiqWatTgtAvgHrMax and ConLiqWatTgtAvgHrAvg, all variables belong to the standard output of TOXSWA (see Section 3.3.13 in Beltman et al., 2018).

Several additional files are produced, including "diagnostics.csv", which provides diagnostic information about the simulation runs, and worker log files ("worker_X.log") providing information on the actions of each worker in case multiple CPUs are used. These files are not further described here, but can be useful for tracking computing time and troubleshooting in the case a run fails to complete.

Table 6   *Attributes of the output file which is produced per reach (csv format). An attribute is only given in the output when it is indicated as requested output in the config file.*

Column header	Description	Format	Example
Timestep	Time step (d)	Float	0.042
Date_time	Date-time stamp	"yyyy-mm-dd hh:mm:ss"	1992-01-01 00:00:00
ConLiqWatTgtAvg_XXXX	Average of momentaneous in target stretch at this time (g.m^{-3})	Float	1.2365
ConLiqWatTgtAvgHrMax_XXXX	Maximum of past hour of average of momentaneous in target stretch (g.m^{-3})	Float	1.2365
ConLiqWatTgtAvgHrAvg_XXXX	Time weighted average of past hour of average of momentaneous in target stretch (g.m^{-3})	Float	1.2365
CntSedTgt1_XXXX	Total content in target layer 1 of sediment (g.kg-1) at this time	Float	1.2365
MasWatLay_XXXX	Mass in water layer (g) at this time	Float	1.2365
MasDrfWatLay_XXXX	Mass entered in water layer by spray drift (g) for past hour	Float	1.2365

---

[4]   Some other output files, including plots can be produced, but since these are not crucial, they are not described here.

Column header	Description	Format	Example
MasSedInWatLay_XXXX	Mass penetrated into sediment from water layer (g) for past hour	Float	1.2365
MasSedOutWatLay_XXXX	Mass transferred from sediment into water layer (g) for past hour	Float	1.2365
MasDwnWatLay_XXXX	Mass flowed across downstream boundary out of water layer (g) for past hour	Float	1.2365
MasUpsWatLay_XXXX	Mass flowed across upstream boundary into water layer (g) for past hour	Float	1.2365
MasTraWatLay_XXXX	Mass transformed in water layer (g) for past hour	Float	1.2365
MasVolWatLay_XXXX	Mass volatilised from water layer (g) for past hour	Float	1.2365
MasSed_XXXX	Mass in sediment (g) at this time	Float	1.2365
MasTraSed_XXXX	Mass transformed in sediment (g) for past hour	Float	1.2365
DepWat	Depth of the water layer at this time	Float	1.2365
VelWatFlw	Flow velocity of water at this time	Float	1.2365
QBou	Discharge at this time	Float	1.2365

3.5   TOXSWA kernel

For each reach the CASCADE-manager sets up a run. In this set up the TOXSWA input file names are based on the names of the reaches listed in the Reaches.csv. From this file also the connections to other reaches, i.e. the names of the upstream reaches and the downstream reach are read and written to the ReachID.txw file.

The folder structure is given in Chapter 4.

3.5.1   Input files for the TOXSWA kernel

As indicated in Section 3.2 there are three types of input files per run, i.e. the hydrology file (hyd), the fate file (txw) and the timestep mass flux file (mfs). For the attributes and format requirements of the hyd and the txw file we refer to Beltman et al. (2018). The mass flux time step file (RunID.mfs file) is new. The file is made for all reaches in the catchment not being a so-called first reach, i.e. a reach that has no upstream reaches. The attributes of this file are given in Table 7. In the file for each hour the mass flux time step is given. This time step is calculated using the procedure described in Annex 1.

Table 7   *Attributes of the mass flux timestep file (mfs).*

Variable	Units	Format	Column header
Time	days	Standard, prec. 0.001 d	Time
Date-time	-	dd-MMM-yy-hhhmm	Date
Time step	s	Standard, prec. 0.01 s	Mass flux time step

```
Example mass flux time step file

*  Time          Date   Mass flux time step
*  (-)           (-)            (s)
   0.000 01-Jan-07-00h00   600.
   0.042 01-Jan-07-01h00   0.05
   0.083 01-Jan-07-02h00   2.
   0.125 01-Jan-07-03h00   60.
```

3.5.2   Output files (for exchange between reaches)

During the run TOXSWA makes a mass flux file, ReachID.mfu, giving the mass flowing out of the reach. The time step for which this output is given differs per hour, and is read by TOXSWA from the mass flux time step (mfs) file of the downstream reach. The format and an example of the ReachID.mfu file is given below. In the example in the first hour the mass flux time step is 600s; hence mass fluxes of 6 steps are given, in the second hour the mass flux time step is 0.1 s, hence mass fluxes of 36000 steps are given. The minimum value for the mass flux time step is set to 0.1 s.

Table 8   *Attributes of the mass flux file (mfu).*

Variable	Units	Format	Column header
Time	days	Standard, prec. 0.000000001 d	Time
Date-time	-	dd-MMM-yy-hhhmm:ss:mmm	Date
Mass flux	g	scientific, ≥3 sig. digits	Mass flux

```
Example mass flux file

*  Time              Date                 Mass flux
*  (-)               (-)                     (g)
   0.000000000   01-Jan-07-00h00:00:000 0.000E+00
   0.006944444   01-Jan-07-00h10:00:000 3.221E-03
   0.013888889   01-Jan-07-00h20:00:000 3.284E-03
   0.020833333   01-Jan-07-00h30:00:000 3.322E-03
   0.027777778   01-Jan-07-00h40:00:000 0.000E+00
   0.034722222   01-Jan-07-00h50:00:000 0.000E+00
   0.041666667   01-Jan-07-00h60:00:000 0.000E+00
   0.041667824   01-Jan-07-00h60:00:100 0.000E+00
   0.041668981   01-Jan-07-00h60:00:200 0.000E+00
   0.041670139   01-Jan-07-00h60:00:300 0.000E+00
```

During the run TOXSWA reads the mass fluxes of its direct upstream reaches. Generally, one reach is situated upstream, but more reaches can discharge into a reach. All directly linked upstream reaches read the required mass flux time step from the ReachID.mfs file of the current reach; so all mfu files of the (directly linked) upstream reaches use the same mass flux time step. In the simulation of the reach, TOXSWA sums the mass fluxes of the upstream reaches to one mass flux entering the reach. A split up of masses over two or more downstream reaches is not (yet) possible.

When there is no upstream reach, the mass flux entering is zero. When there is no downstream reach the mass flux time step applied is 3600 s.

4 Running CASCADE_TOXSWA

The CASCADE_TOXSWA module includes a self-contained Python environment, including all necessary packages, located in "WPy64-3760\" in the module root directory. Before running the module, the environment should be activated by running the following command form the module root directory in a command prompt window:

> WPy64-3760\scripts\env.bat

Then the module is run, again from its root directory, with the following command:

> python src\TOXSWA_IFEM.py <configFile>

Where <configFile> is the name of the configuration file, e.g. "IFEM_config.ini".

CASCADE_TOXSWA will create a directory for the simulation in the module root directory named "experiments\<experimentName>", where <experimentName> is the name of the simulation experiment specified in the configuration file. The results of the simulation will be put in this directory.

The TOXSWA working directory is located in "experiments\<experimentName>\work"

Based on the "Expsd" variable in the reach specification file (specifying whether a reach receives drift input, see Table 2), the module determines whether or not a reach receives substance input at any time during the time period of the input data, either from drift or from its upstream reach(es). If this is not the case, no simulation is performed, and a "dummy" output file is generated, containing zeros for all variables and time steps. This is indicated on the screen. Note that the simulation need not be performed for the full period of input data in the hydrology and mass loading files. This is specified by parameters startDateSim and endDateSim in the configuration file. Hence, it is possible that for a given reach no drift input occurs in the simulation period, even though this reach has value "True" for variable "Expsd".

5 Relevant concepts for future versions of CASCADE_TOXSWA

The current version of CASCADE_TOXSWA is developed for the drift deposition entry route only. In next versions have to be added lateral entries of water and substance by drainage, runoff and erosion. The TOXSWA kernel already simulates lateral entries. These additions need to be made to allow these lateral entries in a landscape scale situation.

The current version simulates substance transport based on advection only. Each reach is considered as ideally mixed. In future versions segmented water layers are recommended to allow to simulate dispersion transport within reaches. Simulation of dispersive transport between reaches is more elaborate and will require concept development.

The simulation of dispersive transport demands increased computation efforts. Therefore, it is recommended to explore options for reducing simulation times. Possible options to explore are the simulation of fewer sediment subsystems of segmented reaches or smart optimisation techniques that make use of e.g. MPI (message passing interfaces).

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Annex 1 Technical description of residence time dependent time steps for mass flux between reaches for CASCADE_TOXSWA

For CASCADE_TOXSWA the time steps for mass flux between reaches is based on the residence time of the water in the reach. The mathematical concept and technical implementation for the CASCADE-manager and for TOXSWA are described in this annex.

A. Technical procedure for timestep of mass flux between reaches

The procedure is explained for the flux of mass between two reaches (R_i and R_{i+1}) for one hour. The procedure can be applied for flux between all reaches and for all hours.

1. Calculate the wetted cross section of the reach, A (m²), from the bottom width (m), slope s_1 (hor/ver) and water depth (m);

$$A = hb + h^2 s_1 \tag{1}$$

2. Calculate time step for each reach using length or reach (L in m), discharge (Q in m³/s), cross section (A in m²), and factor k (-). Note that $L/(Q/A) = \tau$ (residence time).

$$\Delta t_i = \frac{L_i}{\frac{Q_i}{A_i}} * k \tag{2}$$

3. The hydrology time step t_h, currently 3600 s, has to whole number multiplication of the time step Δt_i. Hence the number of time steps in the hour, n_i, should be;

$$n_i = \left\lfloor \frac{t_h}{\Delta t_i} \right\rfloor + 1 \tag{3}$$

   (floor function: the function that takes as input a real number x and gives as output the greatest integer less than or equal to x)

   Then the time step applied for mass flux is given by

$$\Delta t_i = \frac{t_h}{n_i} \tag{4}$$

The chart in Figure A1 shows how the CASCADE-manager organizes the exchange of mass between the reaches. The steps are:

1. The **CASCADE-manager** determines the time step per reach and per hour using Eqs (1)-(3), and writes these to a file per reach, the ReachID.mfs file.
2. The **CASCADE-manager** writes the reach ID of the downstream reach and the upstream reaches to the TOXSWA input file.
3. **TOXSWA** reads the mass flux time step from the ReachID.mfs of its downstream reach (only single downstream reaches is supported).
4. **TOXSWA** uses this time step to write mass flux over the lower boundary to the mass flux file, the <ReachID>.mfu file. Note; internal TOXSWA calculation time step ≤ mass flux time step.

5. **TOXSWA** reads the upstream mass flux from the upstream reaches using the given IDs. In case there are more upstream reaches that discharge into the current reach, the masses will be added by the TOXSWA kernel. When there is no upstream reach, the mass flux entering is set to zero.
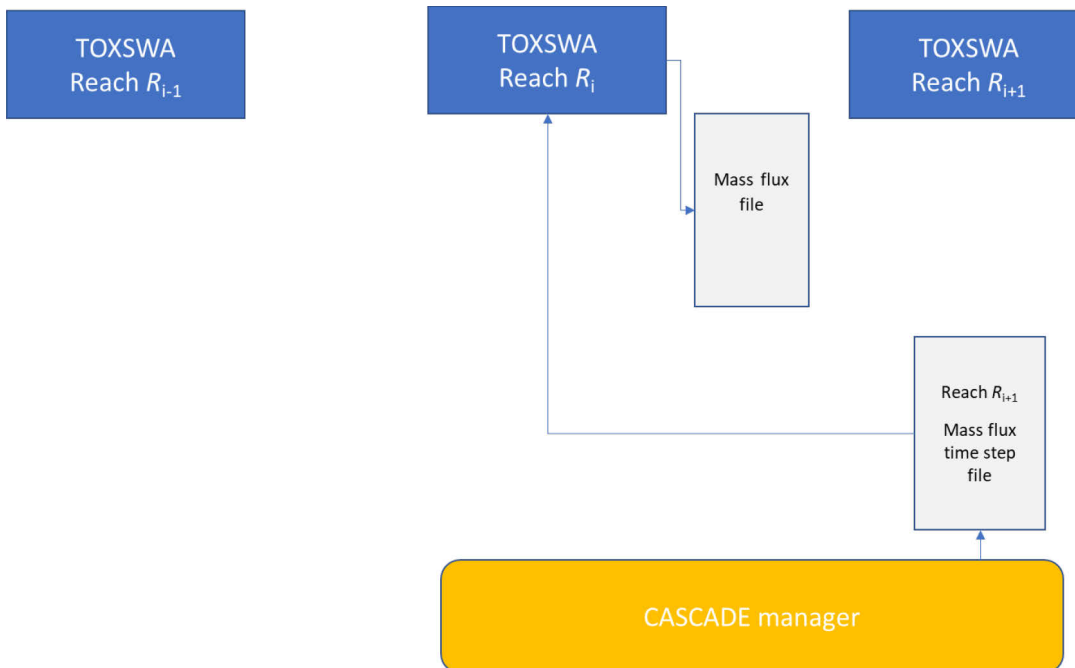

Figure A1 *Chart showing how CASCADE-manager sets up the TOXSWA runs for the reaches.*

TOXSWA is changed to be able to read and write mass fluxes by set time steps for each hour (flexible per hour) instead of hourly values only.

An example of the addition to the TOXSWA input file is shown below; ReachID of upstream reaches and the single downstream reach (info from Reaches.csv file).

```
* Connections to reaches in catchment
* IDs of upstream reaches
Table ReachIDUp
25
28
end_Table
31   ReachIDDwn  (-)  ! ID of downstream reach [1|]
```

An example of the mfu file is shown below. TOXSWA writes required output to this file (see for specifications Section 3.4). The first hour mass flux time step is 600s; hence output of 6 steps, in second hour it is 0.1 s, hence output of 36000 steps.

```
*   Time                Date                Mass flux
*   (-)                 (-)                   (s)
0.000000000   01-Jan-07-00h00:00:000      0.000E+00
0.006944444   01-Jan-07-00h10:00:000      3.221E-03
0.013888889   01-Jan-07-00h20:00:000      3.284E-03
0.020833333   01-Jan-07-00h30:00:000      3.322E-03
0.027777778   01-Jan-07-00h40:00:000      0.000E+00
0.034722222   01-Jan-07-00h50:00:000      0.000E+00
0.041666667   01-Jan-07-00h60:00:000      0.000E+00
0.041667824   01-Jan-07-00h60:00:100      0.000E+00
0.041668981   01-Jan-07-00h60:00:200      0.000E+00
0.041670139   01-Jan-07-00h60:00:300      0.000E+00
.
.
```

Annex 2   TOXSWA main characteristics

This annex provides the main characteristics of the TOXSWA kernel settings. These are fixed in the input template as well as some of the required inputs from the landscape model.

Model science	TOXSWA in CASCADE_TOXSWA	Received from the landscape model	Time dependent?
Compartments/numerical			
Compartments considered	Water, suspended solids, air, plant and sediment		
Compartment segmentation	Segments in water layer set by user; segments layers in sediment and division of layers into sediment segments set by user		
Numerical technique	Explicit		
Numerical dispersion	None *in* reaches, a correction for numerical dispersion is part of the model Between reaches depending on spatial and temporal resolution		
Hydrology			
Method	External, input of hourly discharge and water depth per reach	Time dependent water depth and discharge per reach, drainage water flow, runoff water flow	yes
		Shape of water course, length of reach	no
Pesticide processes water system			
Transport			
Convective transport	Included		
Dispersion	Included		
Diffusion	Not included because significantly small compared to dispersive flux		
Loadings	Spray drift, drainage, runoff	Spray drift,	yes
Width water surface drift entry	At time of drift occurrence calculated from dimensions of reach and water depth		
Sorption			
Environmental conditions	Kf calculated as a function of organic matter content in the suspended solids	Temperature, daily	No
Suspended solids	Freundlich isotherm	Sorption coeffient, Freundlich exponent	No
Macrophytes	linear sorption coefficient	Sorption coefficient	no
Volatilisation	Laminar air boundary layer concept, temperature dependent	Temperature, daily	yes
Environmental parameters	Vapour pressure and solubility adjusted for effect temperature	Vapour pressure, solubility	no
Transformation			
Metabolites	Formation and transformation of metabolites	Formation fraction, metabolite scheme	
Kinetics	First order	Half-life	

Model science	TOXSWA in CASCADE_TOXSWA	Received from the landscape model	Time dependent?
Environmental conditions	Rate coefficient of transformation adjusted for effect temperature	Temperature, daily	yes
Mechanisms considered	Only one process considered (no distinction between biotic and abiotic transformation)		
Pesticide process sediment			
Transport			
Convective transport and dispersion in liquid phase	Not included, therefore dispersion not relevant		
Diffusion in liquid phase	Included		
Exchange between water and sediments layers	Via diffusion		
Sorption			
Environmental conditions	Kf calculated as a function of organic matter content in the sediment layer	Temperature, daily	
Transformation			
Metabolites	Formation and transformation of metabolites considered		
Kinetics	First order		
Environmental parameters	Rate coefficient of transformation adjusted for effect temperature		
Mechanisms considered	Only one process considered (no distinction between biotic and abiotic transformation)		
Pesticide exchange at water-sediment interface			
transport	By diffusion		
Length interface	Based on depth defining perimeter h_w entered by user. Only exchange with sediment below height h_w. h_w must be lower that minimum water depth of simulation.		Proposal for landscape model to use one value for each Strahler order of reaches

Annex 3 Template of TOXSWA *.txw file

The parameters given within <> need to be set by the CASCADE-manager. All other parameters are fixed. The waterbody table (file Section 2 in the *.txw file) is also filled, but does not have a place holder (i.e. <>).

```
* Input file for TOXSWA                                      (c) Wageningen University & Research
*--------------------------------------------------------------------------------------------

table ReachUp
end_table
<downstreamReach>   ReachDwn

*** Section 0: Run identification
Melsterbeek Location
1           WaterbodyID
Pome        CropName
FOCUS       SedimentTypeID
<substanceName>         SubstanceName
Xplcit      ApplicationScheme

*** Section 1: Control
CASCADE     CallingProgram
1           CallingProgramVersion
<startDateSim> TimStart
<endDateSim> TimEnd
Hourly      OptInp
ExtModel    OptHyd
OnLine      OptTem
Calc        OptTimStp  ! Option for time step in mass balance calculation [Input, Calc]
No          OptCalcStabilityWater
No          OptCalcStabilitySediment
<MaxTimStpWat>       MaxTimStpWat (s) ! Maximum calculation time step in water layer [0.001|3600]
<MaxTimStpSed>       MaxTimStpSed (s) ! Maximum calculation time step in sediment [0.001|3600]

* IOMode: options for screen output control, for use for grid computing    (hierover even overleg)
* IOMode_Std    standard screen
* IOMode_Full   full screen
IOMode_Std    IOMode         ! Option selected for screen output [IOMode_Std, IOMode_Full]

*** Section 2: Waterbody
table WaterBody
end_table
11          ConSus (g.m-3)
0.09        CntOmSusSol (g.g-1)
0           AmaMphWatLay (g.m-2)

*** Section 3: Hydrology:
SimpleDitch OptFloWat
WaterCourse OptWaterSystemType
Fischer     OptDis

*** Section 4: Sediment
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
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)
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


*** Section 5: Weather
temperature.met MeteoStation
DailyAir OptMetInp

*** Section 6: Temperature

*** Section 7: Substance
table compounds
end_table
table FraPrtDauWat (mol.mol-1)
end_table
table FraPrtDauSed (mol.mol-1)
end_table
<substanceProperties>

*** Section 8: Loadings
MFU       OptLoa
Yes       OptLoaStr
table Loadings
end_table

*** Section 9: Initial and boundary conditions for mass balance equations
0          ConSysWatIni (g.m-3)
table interpolate CntSysSedIni (mg.kg-1)
end_table
0          ConAir (g.m-3)
0          ConWatSpg (g.m-3)

*** Section 10: Output control
No        OptDelOutFiles
DaysFromSta  DateFormat
e14.6     RealFormat
Hour      OptDelTimPrn
No        PrintMasStrTgt
0.01      ThiLayTgt1 (m)
No        OptOutputThiLayTgt2
All       OptOutputDistances
None      OptOutputDepths
table HorVertProfiles
end_table
DutchRegistration OptReport
Yes       ExposureReport
0         InitYears (-)
No        PrintCumulatives
<outputVariables>
```

Annex 4 Illustration of different types of concentration for understanding movement of mass through the catchment

These slides below were presented to the project group on the development of the landscape scale model (Aquatic Risk@landscape scale project), December 2020. They show first the effect of using a timestep which depends on the Courant number for three single reaches in an example catchment, which is the Rummen catchment in Belgium and an example substance with no exchange with the sediment layer (slide 1-4).

Improved mass transfer and options for linking exposure to effects

- Due to high flow velocities in catchment time resolution used in Cascade_TOXSWA for mass transfer between reaches of 1 hour too course

- Improved numerical solution, by applying Courant number criterium

- Type of output of exposure concentration – how to link to effect

Time step for mass exchange

- Flexible frequency of exchange in CASCADE TOXSWA based on the Courant number:

$$\Delta t = \frac{L}{v} * k$$

L = length or reach (m)

v = flow velocity (m/s) (note that L/v = residence time)

k = scale parameter (-)

Note: we remain with the frequency of 1 hours for the water depth and the discharge
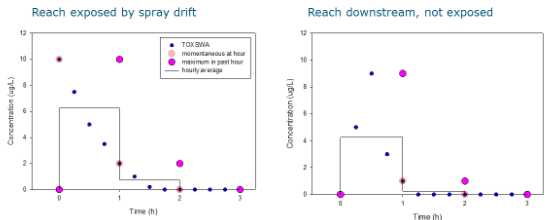
Sub-catchment 20 reaches Strahler order 1 with tracer (and no ex change with sediment)

Mass flux entering reach in g/s   Concentration in reach in ug/L

Old: mass exchange time step 1 hour: dashed line and triangels
New: mass exchange time step < 1 hour (k = 1): solid line and dots
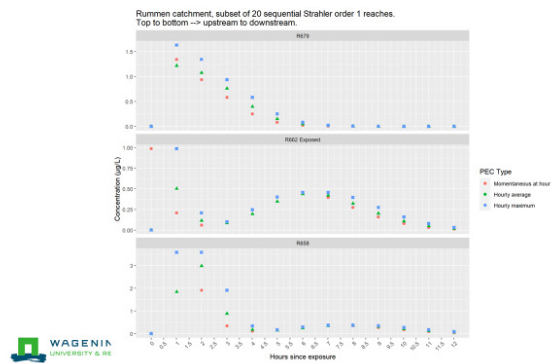
Sub-catchment 20 reaches Strahler order 4 with tracer (and no ex change with sediment)

Mass flux entering reach in g/s   Concentration in reach in ug/L

Old: mass exchange time step 1 hour: dashed line and triangels
New: mass exchange time step < 1 hour (k = 1): solid line and dots

Slide 5-8: In a second part a comparison is made between the three types of output concentrations that can be selected, i.e. momentaneous at the hour (currently used in the FOCUS scenarios), the maximum within te hour, the hourly averaged concentration.
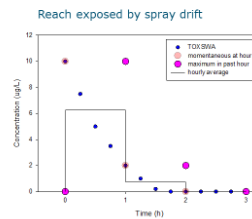
In the third part (slide 9-13) a comparison is made between the three types of output concentrations for the entire catchment (again Rummen catchment).
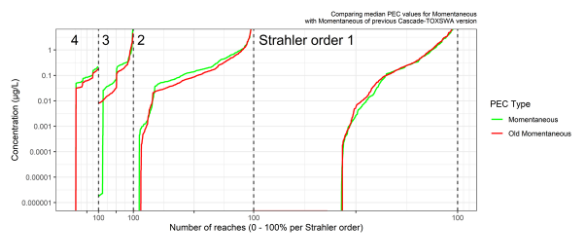
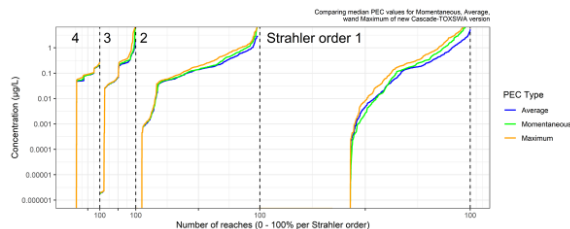## Improved numerical solution

Strahler order 3, 1993; peak, sorted by momentaneous new
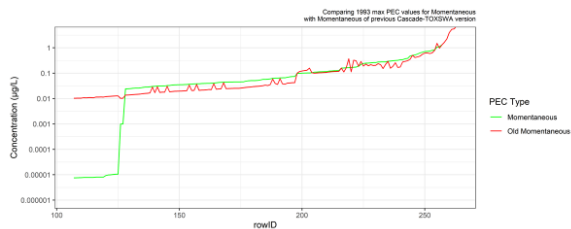
- Momentaneous concentration new mostly higher than old (mass moves faster through system, less dilution), but sometimes lower
- Note that first 28 reaches much lower, due to unwished reboot of PC

Maximum in past hour and average of hour

Strahler order 3, 1993; peak, sorted by momentaneous new

- Maximum concentration sometimes higher (peak occurs in hour), mostly equal to momentaneous (exposed and mixing along travel)
- Average sometimes lower (exposed reaches) and sometimes higher (peak occurs in hour)

Maximum in past hour and average of hour

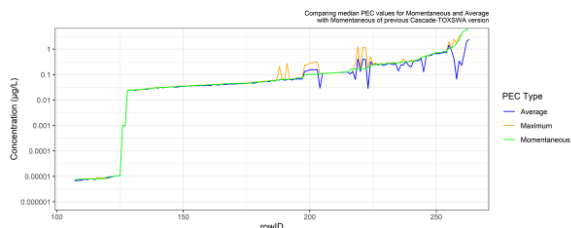Deltamethrin whole catchment 1993-1997; median of peaks of 6 years

- Strahler order 1-4:   maximum ≥ momentaneous
- Strahler order 1:   average < or > momentaneous
- Strahler order 2-4:   average < momentaneous

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