Water quality and aquatic ecology modelling suite

D-Emissions

Deltares systems

User Manual

Deltares

D-Emissions

Assessment tool for the emitted pollution at catchment scale

User Manual

DEM

Version: 7.00
Revision: 00

16 July 2024

D-Emissions, User Manual

Published and printed by:
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1 Guide to this manual

1.1 Introduction

Emission modelling has a long history within Deltares. After very early trials for nutrients (NitSol, PhoSol) in the 1980s, generic approaches started with the development of the Waste Load Model (WLM) in the late 1990s, mostly in international projects like the NWRP in Egypt. This tool was abandoned in the 2000s, although it still remains as a module in Sobek 2. A dedicated emission model was developed for the Marina Reservoir project in Singapore around 2005. In the 2010s a more generic Emission Model (EM) was developed, co-financed by regional water management organizations in The Netherlands. This tool was applied to the Punggol-Serangoon catchment in Singapore, and to some regional water systems in The Netherlands.

When the question came in 2017 to upgrade the dedicated emission model for the Marina Reservoir, a new approach was chosen, inspired by lessons learned in the SOLUTIONS EU FP7 R&D project. This concept had already proven to be practically useful for setting up an emission model for Tire and Road Wear Particles (TRWP, a kind of micro-plastics) (Unice et al., 2019). A new emission modelling approach was created and first applied to the Marina Reservoir Catchment in Singapore in a project for the Public Utilities Board (Deltares project 11201775). The new approach was called “D-Emissions” from that moment on.

In the following years this approach was applied to various issues: macro-plastics (Indonesia 11203482, Thailand), micro-plastics (Tire Industry Project 11203572), chemicals (SOLUTIONS 1209104; DanubeHazard m3c 11204121), “classical” parameters like coliform bacteria and nutrients (Peru WQ assessment 11205177) and “proxies” for pressures on water systems stemming from different land uses (Peru WQ assessment 11205177) (NOTE: The list of projects and project numbers is not exhaustive.)

The final development of D-Emissions into a generic tool has been completed in the DOORS project in 2023 (11207320). It took a longer period because some earlier design choices did not work out well and had to be reversed. This report documents the current status of the generic tool that D-Emissions has become since 2017.

The generic version of D-Emissions can currently be applied in combination with two hydrology models: (1) WFLOW and (2) Hype. The former is an open source gridded hydrology model by Deltares, the latter a partly open source lumped hydrology model by SMHI of Sweden. This manual focuses on the application based on WFLOW. An early version of D-Emissions has been linked to Sobek 2. This version has been documented in project-specific reports.

2 D-Emissions modelling methodology

2.1 System boundary of an emission model

An emission model (EM) has as its main objective:
to quantify "emissions": fluxes of selected substances towards a water system of which the water quality is simulated by a water quality model

To perform this task, the emission model covers a collection of "compartments": parts of the natural environment and the "techno-sphere" (the man-made environment) that are not included in the water quality model.

It is noted that the pathways from the soil system to the surface waters are represented inside D-Emissions.

2.2 Definitions

The key terminology used in the following methodology and used throughout the manual is summarised in Table 2.1 for reference.

Table 2.1: Definition of key terminology

Term	Meaning
Emission	A release of one or multiple substances to a water system included in a water quality model
Compartment	Part of the emission model domain that represents a part of the environment or a part of the "techno-sphere" (the man-made environment); an EM compartment is by definition not part of the water quality model it connects to
Source	An activity or process that generates substances and releases them in any of the EM compartments
Release	Quantity of substances generated by a source
Emission variable (EV)	Variable that explains the release, optionally a function of space and/or time (for example: total area of cleaned buildings)
Activity rate (AR)	Same meaning as EV
Emission factor (EF)	Number expressing the releases of substances per unit of the "emission variable" (for example: detergent use per m2 building cleaned).
Locator (variable)	Spatial variable that drives the spatial distribution of the released mass (can be identical to a space dependent emission variable) (for example: size and location of buildings)
Receptor	Compartment where a source releases mass
Flux	Mass flow (mass per time)
Pathway	The trajectory of the substances released through the compartments of the EM
Treatment	Reduction of substance mass in a compartment through human intervention (for example: a waste water treatment plant)
Retention	Reduction of substance mass in a compartment caused by natural processes (for example: binding of detergent to soil)

2.3 Guiding principles

Many water quality problems related to environmental quality and health can be traced directly to point and diffuse pollution sources. Therefore, emission modelling is often the starting point for many modelling studies related to water quality or health. While traditional water quality models provide insight into the effects of pollutant loads on water systems, the pollution sources themselves are generally described only as conditions at discrete points along the boundary of the model. Identifying and quantifying these conditions is often difficult, especially in the case of diffuse pollution sources, in settings where a number of sources are combined, or where data is lacking to adequately attribute pollution to its source(s).

D-Emissions is intended to organize and quantify assessments of pollution and emissions to water as a stand-alone application or in combination with other tools for more integral analyses of water quality for environmental and human health.

D-Emissions is developed as a tool for emission modelling that is generic enough to be applied in an unlimited number of domains but with sufficient detail of processes common to emission modelling, regardless of spatial scale and data-availability. As such, it facilitates projects in both data-scarce and data-rich contexts.

The guiding principles of the D-Emissions can be formulated as follows:

- ◇ Use relevant socio-economic drivers as input. This will create a true cause-effect chain, provides predictive power and allows for "what if" scenarios driven by policy projections and implemented measures.
- ◇ Use a mass balance-based approach to avoid double-counting or omitting of relevant (parts of) emissions.
- ◇ Provide a consistent link to hydrology: annual loads should respond to inter-annual hydrology variations, and load distribution within the year should be consistent.
- ◇ Provide a consistent representation of relevant pathways, like the pathway from paved surfaces to surface water and the pathway from unpaved surfaces to surface water, dependent on surface runoff, shallow groundwater dynamics and on land-use which determines surface loads to the top-soil.
- ◇ Provide flexibility with respect to compartments, hydrological processes, substances and sources.

2.4 Overall modelling approach

The approach consists of the following basic steps:

- ◇ calculation of release of substances;
- ◇ spatial distribution of the releases of substances;
- ◇ allocation of the releases to certain receiving compartments ("receptor");
- ◇ quantification of pathways to the final destination of the released substance ("emission" to the water quality model) through the compartments of the EM, using hydrological information provided by a supporting hydrological model.

The source oriented approach allows easier calculation of policy scenario's (reduce cows per hectare, reduce farm area, use urine inhibiters, etc.), gives more direct insight where pollutants are coming from, and allows for a better realism check (are we missing a source?, is a source wrongly allocated?, etc.).

Within every schematization element, a calculation procedure as shown in Figure 2.1 is carried out. The emission model is formulated in terms of mass flows. It is implemented within the generic open source water quality modelling software Delft3D. This generic framework takes care of input, output and the compilation of mass balances. Dedicated processes from the Processes Library provide the emission modelling algorithms.

Note that the topsoil and shallow groundwater compartments ("Soil System") are represented within the emission model. Note also that a connected water quality model is supposed to simulate the in-stream transports and processes in surface waters.

2.5 Emission Model

The first step of the emission modelling is the estimation of the releases of target substances and the allocation of these releases to various receptors. These releases are then further routed through the wastewater and stormwater management systems by the emission model, and transformed into total emissions to surface waters (Figure 2.1).

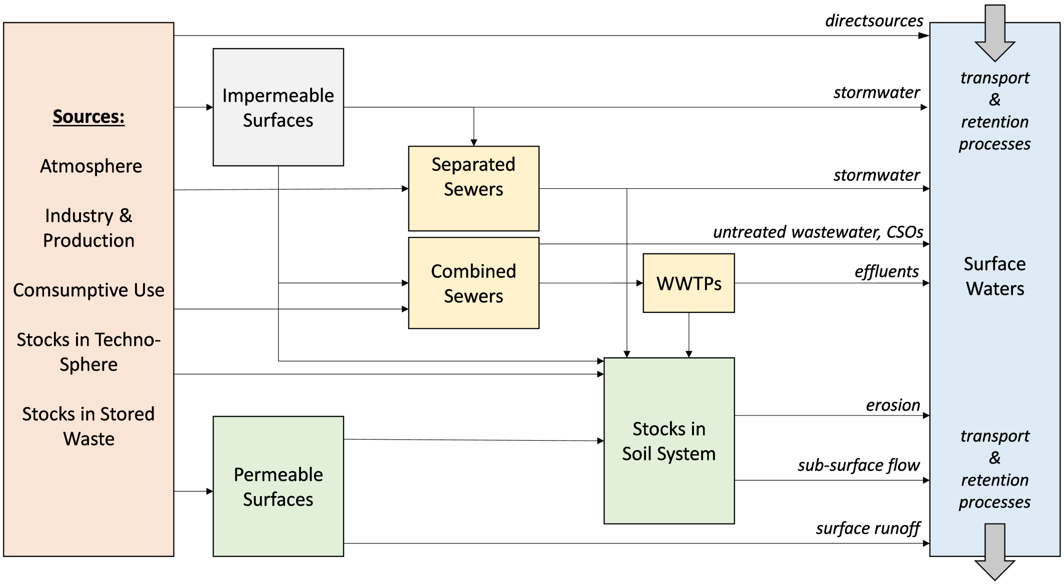

Figure 2.1: *Set-up of the emission model system*

2.5.1 Sources

This approach to emission modelling is "source oriented", as discussed in the related Water Framework Directive Common Implementation Strategy Guidance Document (European Commission, 2012). The definition of sources follows this guidance (Figure 2.2). The essential advantage of this approach is that it provides insight in the origin of the emissions. Therefore, it provides essential information for the definition of emission reduction measures. Atmospheric deposition, though actually a pathway, is seen as a source. The interpretation towards the underlying true sources needs to be provided by expert judgement.

The quantification of the releases of substances associated to the various sources proceeds by the emission factor method. A variable collection of sources can be considered. Releases (L) of a pollutant "p" for a certain socio-economic activity "a" are calculated by multiplying an activity rate (AR_a) by an emission factor for this activity and a certain pollutant ($EF_{p,a}$):

Releases are distributed in space according to two alternative methods:

- ◇ The activity rate is known for a larger geographic area (region, country). The releases are first calculated at this aggregated level and then distributed in space using an auxiliary spatial variable called a "locator".
- ◇ The activity rate is already a spatially distributed variable and can be directly used to calculate spatially variable releases.

The quantified releases are allocated to various initial receptors and routed towards the final receiving surface water compartment (as shown in Figure 2.1). Initial receptors can be: domestic wastewater, the surface waters (directly), the soil system (directly), impermeable

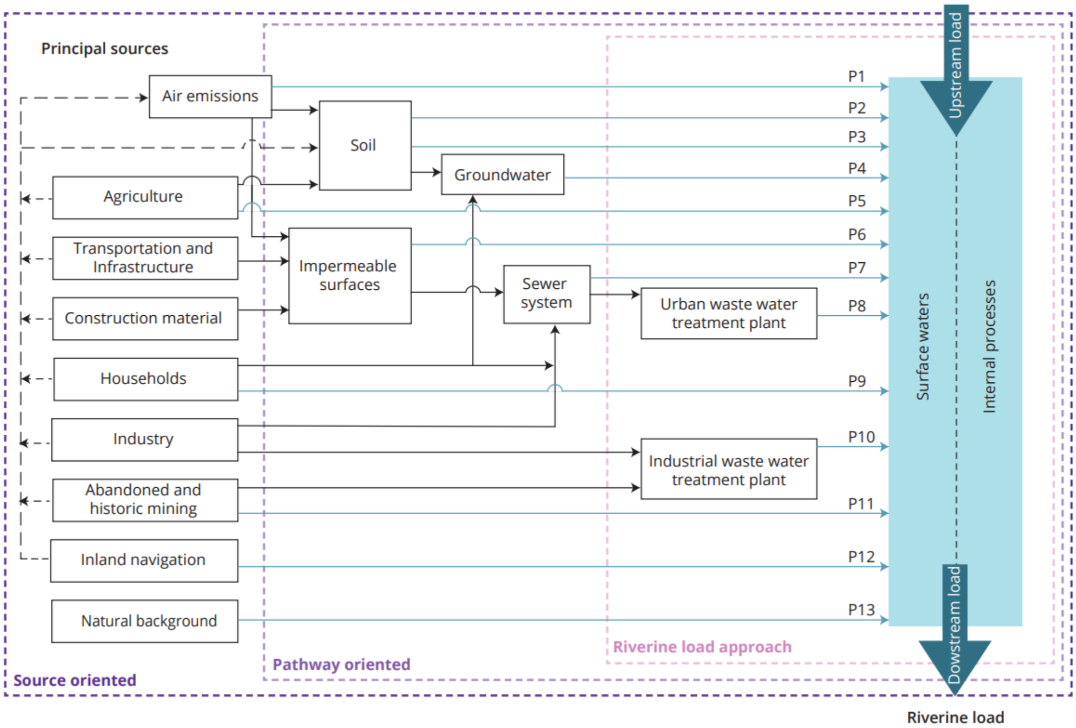

Figure 2.2: *Schematic representation of source-oriented approach towards emission modelling and key pathways (scheme from European Commission (2012), in this form copied from EEA (2018)).*

surfaces, permeable surfaces, the sewage collection system (combined or separated) and the separate rainwater collection system.

2.5.2 Pathways: Stormwater and wastewater

The emissions related to stormwater and wastewater are simulated as follows:

- Domestic wastewater is considered an initial receptor receiving wastewater from households. Depending on the wastewater management infrastructure, the wastewater is routed to the sewer system, to surface waters or soils. This takes into account the share of unconnected households and the share of households using septic tanks or other “individual or appropriate systems” (IAS, as defined under the Urban Wastewater Treatment Directive).
- The substances washed off from impermeable areas find their way to a separate rainwater collection system, a combined collection system for stormwater and wastewater or to surface waters and soils in places where there is no collection system.
- Separate collection systems discharge to surface waters, while a retention term can be defined that is partly allocated to soils (re-use or distribution of sludge).
- Combined collection systems discharge via a WWTP, where the treatment level can be variable.
- Combined collection systems feature overflow events (CSOs), during which the treatment is bypassed; CSOs are a prescribed fraction or occur if a daily rainfall threshold is exceeded.

2.5.3 Pathways: Permeable surfaces

As discussed above, all pathways related to the soil system are simulated within D-Emissions. The emission model has a "permeable surfaces" compartment and an underlying "soil" compartment. A relevant consideration is that the permeable surfaces compartment in EM can be configured to have a short "residence time". It responds rapidly to hydrological events, unlike the soil system.

For applications connected to a distributed model (like WFLOW) the following considerations hold:

- The emission model is implemented on the full grid.
- The grid cells are marked as "river" or "land".
- Substances are routed through the grid and the various compartments as dictated by the hydrology.
- Horizontal transports (i.e. between connected grid cells) occur by overland and subsurface flows.
- The mass that arrives in the surface water compartment of a river cell constitutes the "emissions" to that cell, is taken out of the emission model and passed to the water quality model.
- Consequently, the water quality model only covers the river cells.

2.6 Link to water quality models

D-Emissions runs on a substance-by-substance basis. If the WQ model requires emission estimates for different substances (for example both nitrogen and phosphorus), multiple runs of D-Emissions are required. Within the WQ model, dedicated processes are available in the processes library to pick up the emissions and, if relevant, distribute them over different WQ model state variables (for example PON1, NH4 and NO3 for nitrogen, POP1, PO4 and AAP for phosphorus.

2.7 Input data

2.7.1 Schematization

D-Emissions uses a spatial representation of the model domain. This representation is "unstructured", meaning that there is no prescribed alignment of the schematization elements. The schematization is normally derived from an underlying hydrology model. D-Emissions has been coupled to both lumped hydrology models (example: Hype, Figure 2.3) and distributed hydrology models (example: WFLOW, Figure 2.4).

A lumped model consists of irregularly shaped sub-catchments embedding both land and water. The schematizations of D-Emissions and D-Water Quality both cover all sub-catchments. For a distributed model, the D-Emissions implementation works on all cells (land and river). It calculates emissions to river cells only, anticipating a water quality model that consists of the river cells. Horizontal transport between land cells is arranged within D-Emissions.

Spatial input needs to be provided by the user, simply as a list of numbers for the schematization elements distinguished by the hydrology model. The associated GIS operations are left to the responsibility of the user.

It is noted that a standard coupling is available between WFLOW and D-Emissions model, and also between WFLOW and D-Water Quality.

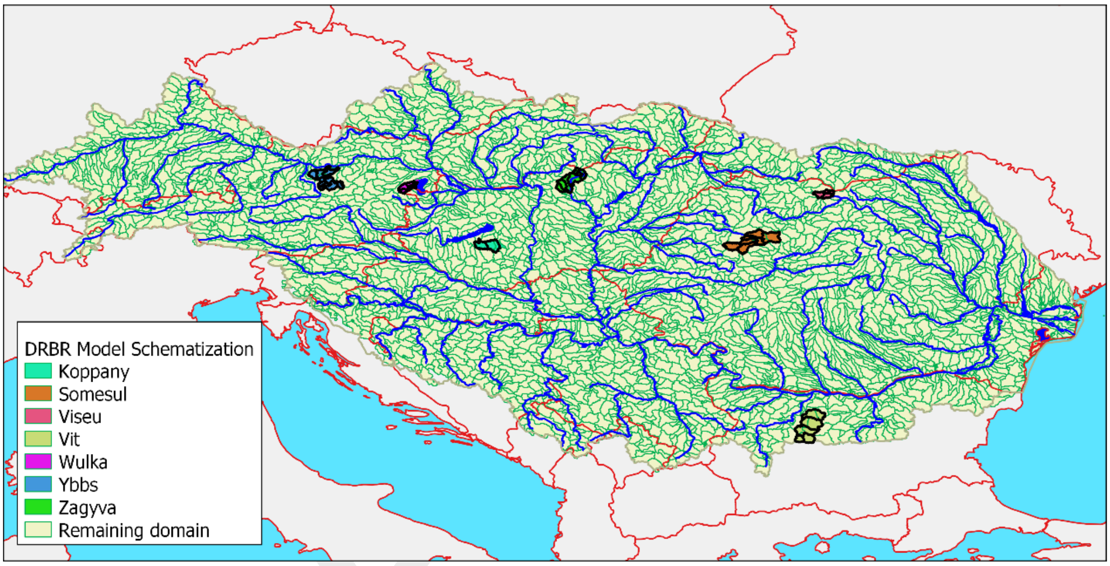

Figure 2.3: *Example of a D-Emissions schematization based on a lumped hydrology model (example for the Danube River Basin, using Hype).*

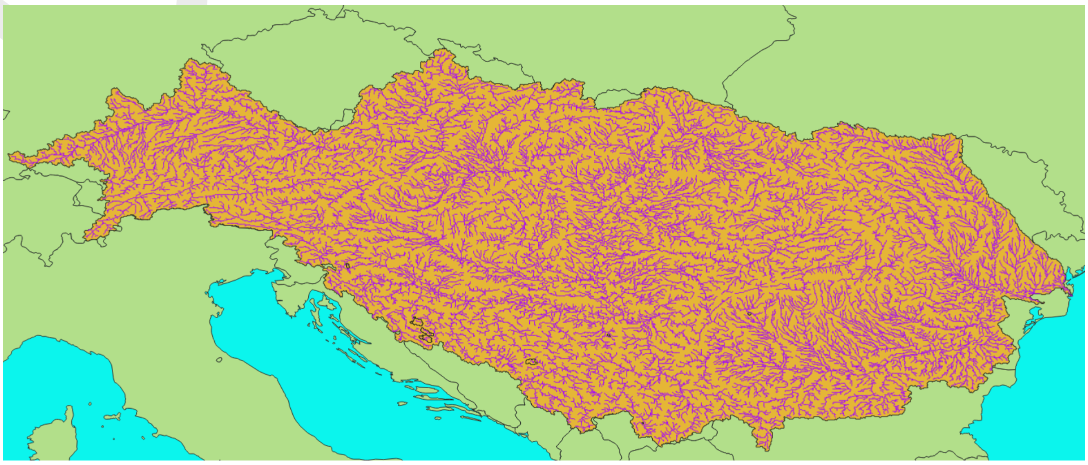

Figure 2.4: *Example of a D-Emissions schematization based on a distributed hydrology model (example for the Danube River Basin, using WFLOW). Land cells are green in the plot, while river cells are blue.*

2.7.2 Emission variables or activity rates

Releases of substances are estimated as indicated in Section 2.5.1. There is no restriction as to which input can be used to estimate releases. Relevant examples are population numbers or specific land uses.

2.7.3 Land-use

Selected land-use information plays a role in the emission modelling. The current implementation presumes that a coupling is in place to a hydrology model that provides information on paved area (impermeable), unpaved area (permeable) and open water area.

2.7.4 Hydrology

Selected land-hydrology information plays a role in the emission modelling. The current implementation presumes that:

- ◇ a coupling is in place to a hydrology model that provides the required input;
- ◇ every schematization element is coupled to a single downstream element;
- ◇ an optional distinction can be made between "land" (only) and "river" (including land) elements.

2.7.5 Sediment delivery to rivers

Optionally, the erosion pathway can be represented using external data on the delivery of fine particles to streams. To this end, a link is available to the sediment model embedded in WFLOW.

2.7.6 Wastewater and stormwater management infrastructure

Emission modelling depends considerably on information about the available wastewater and stormwater management infrastructure. This concerns for example the presence of collection systems and the presence and efficiency of treatment. Details will be evident from the chapters that follow.

3 Detailed functional description

3.1 Introduction: Generic Single Substance Emission Model (EM_GSS)

The emission modelling process quantifies releases to various compartments and routes them to the surface waters. It is applied for a single substance.

Releases are defined for:

- ◇ Atmospheric deposition: dry deposition as mass/time/surface area, wet deposition as mass/volume in precipitation;
- ◇ A variable number of “type A” sources;
- ◇ A variable number of “type B” sources.

See Section 2.5.1 for an explanation of types A and B.

3.2 Implementation

The EM is currently configured for 8 compartments.

Table 3.1: *Eight compartments*

Abbreviation	**Description**
Dww	Domestic wastewater, the wastewater generated by households and small shops and enterprises in cities and villages
Sew	Sewer system that receives wastewater and (optionally) stormwater
Pav	Paved or impermeable surfaces
Unp	Unpaved or permeable surfaces
Stw	Sewer system that receives only stormwater
Sfw	Final recipient surface water, all matter that ends up here is “emissions to surface waters”
Soi	Soil compartment
SoiPass	Second soil compartment that holds an immobile (“passive”) fraction of the simulated substance

In the EM software and input file, these compartments are mathematically represented by substances. The mass of the simulated substances is expressed in grams. “Vertical” transports from one compartment to another in the same schematization element as well as horizontal transports between schematization element (in g/s) are mathematically represented by “process fluxes” (transformations of one substance into another substance). This comes back in the mass balance output.

As the mathematical concept of a “substance” is used to represent compartments, EM has been set up to run for one “true” substance at a time.

3.3 Formulation

3.3.1 Releases

Releases of substances are quantified per time step as discussed in Section 2.5.1). Releases from atmospheric deposition are automatically allocated to the proper receiving compartment (paved surfaces, unpaved surfaces and surface waters) depending on the local conditions that follow from the supportive hydrology model. Releases from other sources need to be allocated to the proper receiving compartment by the user.

3.3.2 Domestic wastewater

Releases to domestic wastewater are routed to “downstream” compartments in accordance with the available infrastructure. Wastewater is either collected in a sewer system (*FrSewered*), or in septic tanks (*FrSeptic*) or remains unmanaged (*1 - FrSewered - FrSeptic*).

For the fraction collected in septic tanks, a loss to surface waters (*EffSeptic*) and to soils (*SldSeptic)* can be defined. The remaining part is assumed transported to treatment plants by other means than sewer systems.

From the unmanaged wastewater, a fraction *fOpenWater* is directly routed to surface waters, the remainder to soils.

Thus, the routing of domestic wastewater is:

$$\begin{aligned} WWtoSew &= FrSewered + FrSeptic * (1 - EffSeptic - SldSeptic) \\ WWtoSfw &= FrUnManaged * fOpenWater + FrSeptic * EffSeptic \\ WWtoSoi &= FrUnManaged * (1 - fOpenWater) + FrSeptic * SldSeptic \end{aligned}$$

3.3.3 Paved surfaces

Figure 3.1 shows a schematic overview of the fate of releases to paved areas. Substances reaching paved areas undergo a decay process and can be washed off. The fraction that is not removed by runoff or decay remains in the paved emission pool. Wash-off starts at a lower threshold (2 mm/ d in Figure 3.1) and the removed fraction linearly increases to 100% at an upper threshold (5 mm/ d in Figure 3.1). The thresholds are input parameters.

In formulas:

$$\begin{aligned} f_{runoff} &= max(min(\frac{RO - LT}{HT - LT}, 1), 0) \\ F_{loss} &= k_{paved} M \\ F_{runoff} &= (\frac{M}{\Delta t} + L - F_{loss}) \times f_{runoff} \end{aligned}$$

where:

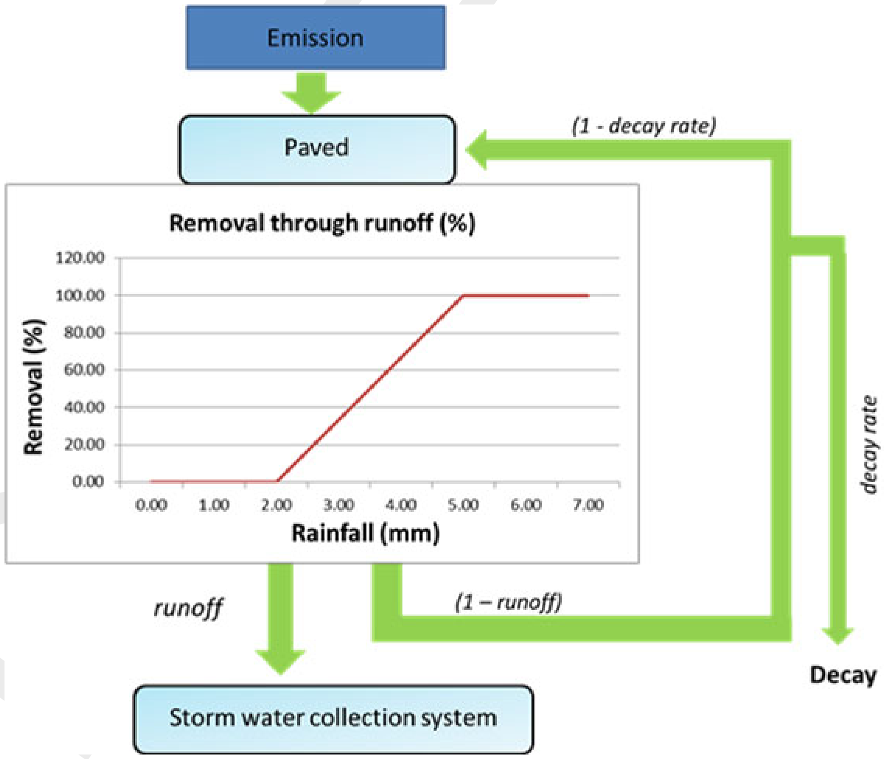

Figure 3.1: *Schematic overview of the pathway that releases follow when distributed to the paved areas. The fate of the release is either runoff to storm water or decay and thereby removal from the model*

f_{runoff}	fraction washed off by surface runoff (-)
RO	actual surface runoff intensity (mm/d)
F_{loss}	flux lost by decay (g/d)
k_{paved}	decay rate (1/d)
M	mass available on paved surfaces (g)
F_{runoff}	flux washed off by surface runoff (g/d)
L	releases to paved surfaces (g/d)
Δt	time step in calculation (d)
LT	runoff intensity for start of mobilization (mm/d)
HT	runoff intensity for complete mobilization (mm/d)

The washed off substances are distributed over different compartments:

- A fraction *FrSewered* is distributed over the*Sew* and *Stw* compartments according to the parameter *fComSew*.
- Out of the remainder, a fraction *fOpenWater* is allocated to *Sfw* and the rest to *Soi*.

3.3.4 Unpaved surfaces

Figure 3.2 presents a schematic overview of the simulated pathways for unpaved areas. The unpaved pool is undergoing burial to the soil compartment and decay. The latter process removes substances from the simulation. Depending on the hydrological conditions, a fraction of the pool can be washed off, infiltrate or erode. The fraction of the emission that is not removed by any of these processes remains in the unpaved pool.

The pool is split into fractions bound and unbound to soil particles (parameter *KdUnpa*). The bound fraction can erode, the unbound fraction can infiltrate and be washed off. Erosion depends on the rainfall intensity and is controlled by a lower and upper threshold (10 and 20 mm^{-1} in the example shown in Figure 3.2). These thresholds are input parameters. Wash-off and infiltration depend on the sum of both fluxes. At an upper threshold (7 mm^{-1} in the example shown in Figure 3.2) mobilization is complete, distributed over wash-off and infiltration in accordance with the hydrological fluxes.

In formulas:

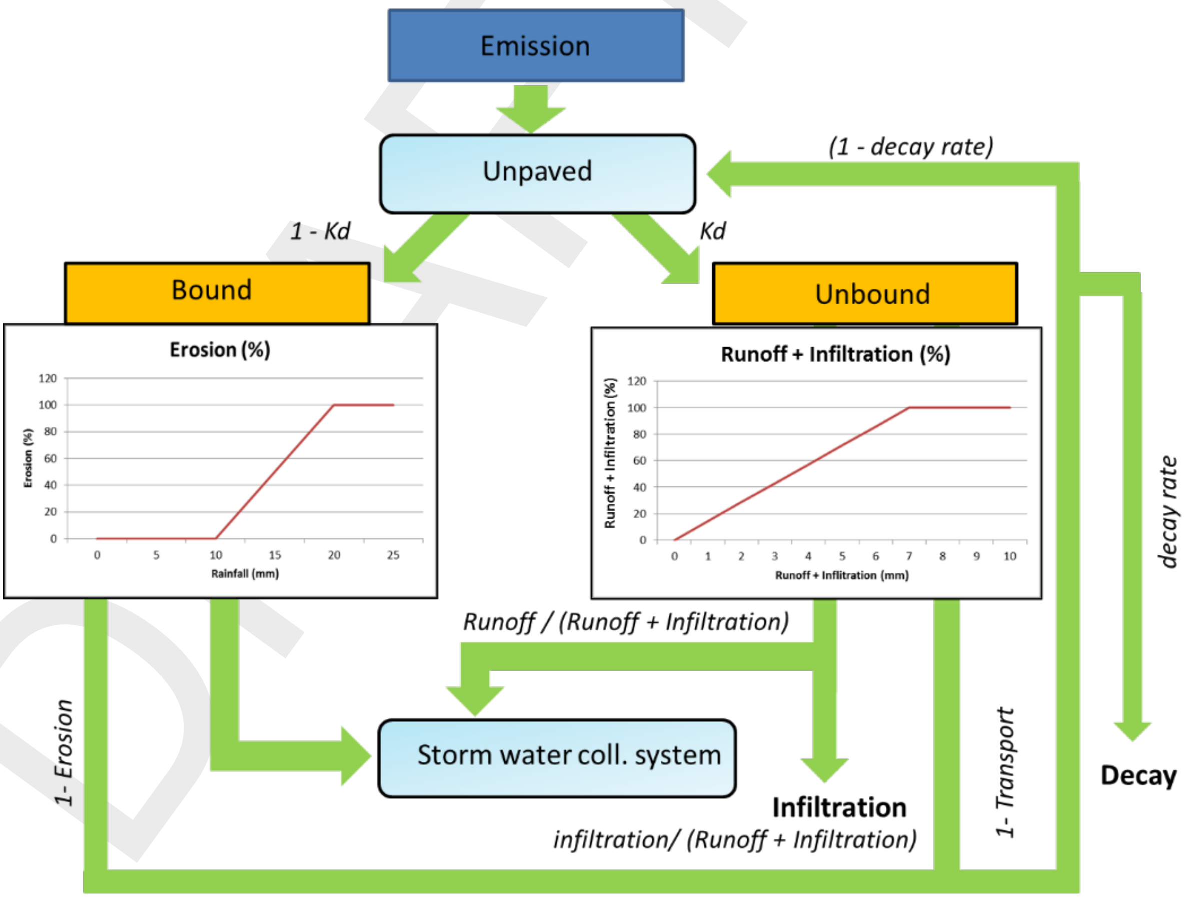

Figure 3.2: *Schematic overview of the pathways in unpaved areas. The releases are first divided over the bound and unbound fractions. The fate of the unbound fraction is either runoff to the storm water collection system (runoff) or infiltration to the soil. The fate of the bound fraction is erosion. Both fractions will experience burial to the soil compartment and decay*

$$f_{erosion} = max(min(\frac{RA - LT}{HT - LT}, 1), 0)$$
$$f_{mob} = max(min(\frac{RO + INF}{7HTM}, 1), 0)$$
$$f_{runoff} = max(min(\frac{RO}{RO + INF}, 1), 0)$$
$$f_{infilt} = max(min(\frac{INF}{RO + INF}, 1), 0)$$
$$F_{loss} = k_{unpaved} \times M$$
$$F_{burial} = b \times M$$
$$F_{dis} = kd_{unpaved} \times (\frac{M}{\Delta t} + L - F_{loss})$$
$$F_{part} = (1 - kd_{unpaved}) \times (\frac{M}{\Delta t} + L - F_{loss})$$
$$F_{erosion} = F_{part} \times f_{erosion}$$
$$F_{infilt} = F_{dis} \times f_{mob} \times f_{infilt}$$
$$F_{runoff} = F_{dis} \times f_{mob} \times f_{runoff}$$

where:

$f_{erosion}$	fraction eroded by surface runoff (-)
f_{mob}	fraction mobilised by runoff or infiltration (-) (-)
f_{runoff}	fraction mobilised by surface runoff (-)
f_{infilt}	fraction mobilised by infiltration (-)
RO	actual surface runoff intensity (mm/d)
RA	actual rainfall intensity (mm/d)
INF	actual infiltration intensity (mm/d)
F_{loss}	flux lost by decay (g/d)
$k_{unpaved}$	decay rate (1/d)
b	burial rate (1/d)
$kd_{unpaved}$	partition fraction (-)
M	mass available on unpaved surfaces (g)
L	releases to unpaved surfaces (g/d)
Δt	time step in calculation (d)
F_{part}	particulate flux available for transport (g/d)
F_{dis}	dissolved flux available for transport (g/d)
$F_{erosion}$	erosion flux by surface runoff (g/d)
F_{runoff}	runoff flux (g/d)
LT	lower rainfall threshold for start of erosion (mm/d)
HT	higher rainfall threshold for complete erosion (mm/d)
HTM	higher threshold for complete mobilisation by runoff and infiltration (mm/d)

The washed off and eroded fractions are routed to the *Sfw* compartment. The infiltrating and buried fractions are routed to the *Soi* compartment.

3.3.5 Combined sewer systems

A flux from the *Sew* to surface water is defined that corresponds to leakages and combined sewer overflows (CSO's). This is controlled by the parameter *SewLeakage*. If this parameter is a positive number, it represents a leakage fraction. If this parameter is negative, it represents a precipitation threshold. If the threshold is exceeded, the inflow to the *Sew* compartment is directly routed to *Sfw*.

The substances remaining in *Sew* may or may not undergo treatment. Up to three different levels of treatment can be distinguished. The remainder is assumed untreated:

$$FrUnTreated = 1 - FrTreat1 - FrTreat2 - FrTreat3$$

For each of the three treatment levels, the fraction of the influent reaching the effluent and the sludge respectively is specified. This implicitly defines the truly removed fraction (not remaining in effluent or sludge). For the complete combined sewers system, the fractions reaching the surface waters without treatment, the treated effluents and the sludge equal:

$$\begin{aligned}
UncWWTP &= FrUnTreated \\
EffWWTP &= FrTreat1 * EffTreat1 \\
&\quad + FrTreat2 * EffTreat2 + FrTreat3 * EffTreat3 \\
SldWWTP &= FrTreat1 * SldTreat1 \\
&\quad + FrTreat2 * SldTreat2 + FrTreat3 * SldTreat3
\end{aligned}$$

In a final step, the fraction reaching sludge is corrected for "removal" of sludge by incineration and isolation. The remaining part is routed to soils.

$$SldWWTPsoils \ = SldWWTP * (1 - fSldgRem)$$

Consequently, the removed fraction equals:

$$RemWW = 1 - FrUnTreated - EffWWTP - SldWWTPsoils$$

Thus, three separate fluxes to surface waters are quantified: by treated effluents, by sewers not connected to treatment plants and by combined sewer overflows.

The definition of an optional parameter*WWreceptor* allows a man-induced horizontal displacement of the treated and untreated effluents (*UncWWTP* and *EffWWTP*) reaching the surface waters. This is relevant in small scale applications, e.g. in cities. (NOTE: This functionality is not yet implemented)

3.3.6 Separated sewer systems

The substances remaining in*Stw* can partly be retained. The fate of the substances in the influent is fixed by the parameters specifying the fractions that end up in effluent (*EffRS*) and in sludge (*SldRS*) respectively. These two parameters implicitly determine the retention (*1-EffRS-SldRS*).

The definition of an optional parameter *SWreceptor* allows a man-induced horizontal displacement of effluents (*Eff_RS*) reaching the surface waters. This is relevant in small scale applications, e.g. in cities. NOTE: This functionality is not yet implemented.

3.3.7 Soil system

The soil system receives substances by direct release, by burial (bound fraction) and by infiltration (unbound fraction) both from unpaved surfaces. In the soil system, two pools are present. Next to the regular (active) soil pool that receives the releases, burial and infiltration, there is a passive soil pool. This passive pool:

- ◇ Represents a separate chemical state of the simulated substance, not directly connected to present releases.
- ◇ Contributes to the erosion flux in proportion to its presence.
- ◇ Contributes to exfiltration and subsurface flow fluxes in proportion to a prescribed concentration.

A relatively simple soil mass balance is compiled. While in the soil system, a decay rate can be specified, as well as an immobilization rate that moves material from the active to the passive pool.

A relatively simple soil mass balance is compiled. While in the soil system, a decay rate can be specified, as well as an immobilization rate that moves material from the active to the passive pool.

The outflow from the active soil pool follows from the simulated concentration in the soil moisture. The outflow from the passive soil pool follows from a prescribed concentration in the soil moisture. The residence time in the soil system is implicitly determined by the soil thickness and soil porosity, in combination with the exfiltration and subsurface flow rates. Outflow from the soil pools is routed to the surface water (exfiltration) or to the downstream cell (subsurface flow).

An alternative erosion process is formulated here, driven by externally determined soil erosion fluxes. The concentration in the eroded particles is calculated by dividing the mass of the simulated substance and the soil dry mass.

In formulas:

$$
\begin{aligned}
F_{loss} &= k_{soil} M_{act} \\
F_{immo} &= k_{immo} M_{act} \\
C_{act} &= \frac{M_{act}}{SoilThick \times SoilPor \times Surf} \times kd_{soil} \\
F_{exf,act} &= C_{act} EXF \\
F_{exf,pas} &= C_{pas} EXF \\
F_{ssf,act} &= C_{act} SSF \\
F_{ssf,pas} &= C_{pas} SSF \\
S &= SoilThick \times (1 - SoilPor) \times Surf \times Fr_{unpaved} \times \rho_{DM} \\
F_{ero,act} &= \frac{M_{act}}{S} \times F_{DM,ero} \\
F_{ero,pas} &= \frac{M_{pas}}{S} \times F_{DM,ero}
\end{aligned}
$$

where:

act	referring to active pool
pas	referring to passive pool
EXF	actual exfiltration (mm/d)
SSF	actual subsurface (horizontal) flow (mm/d)
kd_{soil}	partition fraction (-)
k_{soil}	decay rate (1/d)
k_{immo}	immobilization rate (1/d)
SoilThick	thickness of soil compartment (m)
SoilPor	porosity of soil compartment (-)
Surf	horizontal area (m2)
$Fr_{unpaved}$	fraction of unpaved area (-)
M	substance mass in soil compartment (g)
ρ_{DM}	density of dry soil matter (g/m^3)
S	soil mass in soil compartment (g)
F_{loss}	flux lost by decay (g/d)
F_{immo}	immobilization flux (g/d)
C_{act}	dissolved concentration in active pool (g/m^3)
C_{pas}	concentration in outflow from passive pool (g/m^3)
$F_{exf,act}$	exfiltration flux from active pool (g/d)
$F_{exf,pas}$	exfiltration flux from passive pool (g/d)
$F_{ssf,act}$	subsurface (horizontal) outflow from active pool (g/d)
$F_{ssf,pas}$	subsurface (horizontal) outflow from passive pool (g/d)
$F_{ero,DM}$	soil erosion (g/d)
$F_{ero,act}$	erosion flux from active pool (g/d)
$F_{ero,pas}$	erosion flux from passive pool (g/d)

3.3.8 Horizontal transport by surface runoff

Horizontal transport is applied in the surface water compartment of land only cells by surface runoff to the downstream cell. For this to happen, there needs to be overland flow.

$$f_{mob} = max(min(\frac{OF}{HT}, 1), 0)$$
$$F_{hor} = f_{mob} \times \frac{M}{\Delta t}$$

OF	overland flow (mm/d)
HT	threshold for mobilisation (mm/d)
M	substance mass (g)
Δt	time step (d)

3.4 Input

This section provides a complete listing of all input. Where “Spatial function?” is indicated as “no”, there is no option to specify the related input as a function of space. Any defined spatial variability is neglected; the value for the first cell will be applied model-wide. Similarly, where “Time dependent?” is listed as “no”, any defined temporal variability of the input item in question is neglected; the value for the simulation start time will be applied throughout the simulation.

Note:

- ◇ The above refers to the technical implementation. The fact that a certain input item can be space or time dependent does not mean it has to be or even that it makes sense.
- ◇ Some parameters are substance dependent. The responsibility to define realistic values is left to the user.

3.4.1 Geometry and hydrology

The next input items are typically derived from an underlying hydrology model, as constant spatial fields.

Table 3.2: Geometry and hydrology

Item name	Description	Unit	Spatial function	Time dependent
TotArea	total surface area	(m^2)		No
fPaved	fraction paved	(-)		No
fUnpaved	fraction unpaved	(-)		No[1]
fOpenWater	fraction open water	(-)		No
River	Definition of river (>0) or land (0) schematization elements	(-)		No
Downstream	Definition of downstream cell (only needed if separate land and river cells are defined)	(-)		No

(1) Used during model initialization to derive the fate of wastewater.

The next input items are typically derived from an underlying hydrology model, as time- and space-dependent input.

Table 3.3: Hydrology

Item name	Description	Unit	Spatial function	Time dependent
Rainfall	Rainfall	(m^3/s)		No
RunoffPav	surface runoff from paved surfaces	(m^3/s)		No
RunoffUnp	surface runoff from unpaved surfaces	(m^3/s)		No
Infiltr	Infiltration	(m^3/s)		No
Exfilt	Exfiltration (from soil to surface water)	(m^3/s)		No
Subsurface	Subsurface horizontal flow (only needed if separate land and river cells are defined)	(m^3/s)		No
Overland	Overland horizontal flow (only needed if separate land and river cells are defined)	(m^3/s)		No

3.4.2 Releases

The definition of releases is up to the user.

Table 3.4: *Releases*

Name in model	Definition	Unit	Spatial function?	Time dependent?
EV_A01	emission variable of source A01	(X)		
LOC_A01	locator variable of source A01	(Y)		No
EF_A01	emission factor of source A01 (substance dependent)	(kg/d/X)		No
A01toWW	released fraction to wastewater of source A01	(-)		No
A01toSew	released fraction to mixed sewers of source A01	(-)		No
A01toPav	released fraction to paved areas of source A01	(-)		No
A01toUnp	released fraction to unpaved areas of source A01	(-)		No
A01toStw	released fraction to separated sewers of source A01	(-)		No
A01toSfw	released fraction to surface waters of source A01	(-)		No
A01toSoi	released fraction to soils of source A01	(-)		No
EV_B01	emission variable of source B01	(X)		
EF_B01	emission factor of source B01 (substance dependent)	(kg/d/X)		
B01toWW	released fraction to wastewater of source B01	(-)		No
B01toSew	released fraction to mixed sewers of source B01	(-)		No
B01toPav	released fraction to paved areas of source B01	(-)		No
B01toUnp	released fraction to unpaved areas of source B01	(-)		No
B01toStw	released fraction to separated sewers of source B01	(-)		No
B01toSfw	released fraction to surface waters of source B01	(-)		No
B01toSoi	released fraction to soils of source B01	(-)		No
EV_DDp	dry deposition rate (substance dependent)	(g/m^2/d)		
EF_WDp	wet deposition rate (substance dependent)	(g/m^3)		

3.4.3 Management of wastewater and stormwater

The definition of the wastewater and stormwater management infrastructure is up to the user.

Table 3.5: *Wastewater and stormwater*

Name in model	Definition	Unit	Spatial function?	Time dependent?
FrSewered	fraction wastewater intercepted by sewer systems	(-)		No
FrRainSew	fraction stormwater intercepted by sewer systems	(-)		No
FrSeptic	fraction wastewater to septic tanks	(-)		No
FComSew	fraction of combined sewers	(-)		No
SewLeakage	sewer leakage / CSO definition	(-) or (mm/day)		
FrTreat1	fraction wastewater primary treated	(-)		No
FrTreat2	fraction wastewater secondary treated	(-)		No
FrTreat3	fraction wastewater tertiary treated	(-)		No
Eff_Septic	fraction directly to surface waters for septic tanks	(-)		No
Eff_Treat1	fraction to effluent for primary treatment	(-)		No
Eff_Treat2	fraction to effluent for secondary treatment	(-)		No
Eff_Treat3	fraction to effluent for tertiary treatment	(-)		No
Sld_Septic	fraction directly to soils for septic tanks	(-)		No
Sld_Treat1	fraction to sludge for primary treatment	(-)		No
Sld_Treat2	fraction to sludge for secondary treatment	(-)		No
Sld_Treat3	fraction to sludge for tertiary treatment	(-)		No
FrSldgRem	fraction of sludge removed (not reused)	(-)		No
Eff_RS	Fraction to effluent of rain sewers influent (substance dependent)	(-)		
Sld_RS	Fraction to sludge of rain sewers influent (substance dependent)	(-)		
Population[1]	Population	(cap)		
PCWastWat[1]	per capita production of wastewater	(L/cap/d)		
WWreceptor[2]	Destination of effluents from Sew compartment	(-)		No
SWreceptor[2]	Destination of effluents from Stw compartment	(-)		No

[1]) These items are used to calculate the wastewater volume and subsequent concentration in wastewater.
[2]) Functionality not yet implemented.

3.4.4 Pathways in the environment

The pathways in the environment are defined by the below input parameters. Most will need to be set by the user. Defaults are provided when it is logical. The soil properties are typically derived from the underlying hydrology model.

Table 3.6: *Pathways*

Name in model	Definition	Unit	Spatial function?	Time dependent?
kBurial	burial rate of unpaved pool	(-)	No	No
DecPav	decay rate paved (substance dependent)	(1/d)		
DecUnp	decay rate unpaved (substance dependent)	(1/d)		
KdUnpa	fraction of bound vs unbound, unpaved areas (substance dependent)	(-)		
SoilThick	thickness of soil compartment	(mm)		
SoilPoros	soil porosity	(-)		
DecSoi	degradation rate in soil	(1/d)		
ImmoSoi	Immobilization rate (transfer to passive pool)	(1/d)		
KdSoi	fraction of bound vs unbound in soils (substance dependent)	(-)		
SoilPass	Passive soil store (needs to be a state variable)	(g)		
CBack	Background concentration in soil moisture from passive pool	(g/m^3)		
RhoDM	Density of solid phase	(kg/m^3)		
ro_lothr	run-off from hard surfaces lower threshold	(mm/d)	No	No
ro_hithr	run-off from hard surfaces upper threshold	(mm/d)	No	No
ra_lothr	rainfall mediated erosion lower threshold	(mm/d)	No	No
ra_hithr	rainfall mediated erosion upper threshold	(mm/d)	No	No
disp_hithr	dissolved transport from unpaved pool, threshold for runoff + infilt	(mm/d)	No	No
over_hithr	threshold for transport by overland flow (between surface water compartment in adjacent land cells)	(mm/d)	No	No

3.4.5 External sediment data

The emission model allows for optional input data to quantify sediment delivery to streams by erosive processes.

Table 3.7: *Sediment*

Name in model	Definition	Unit	Spatial function?	Time dependent?
ErodIM1l	Erosion flux of fine sediment fraction 1	(g/d)	No	No
ErodIM2	Erosion flux of fine sediment fraction 2	(g/d)		
ErodIM3	Erosion flux of fine sediment fraction 3	(g/d)		
FacErod	Scale factor for erosion fluxes	(-)	No	No

The WFLOW sediment model can provide these data. It does so for the following fractions:

- IM1: clay with mean diameter 0.002 mm;
- IM2: silt with mean diameter 0.010 mm;
- IM3: small aggregates (sagg) with mean diameter 0.030 mm.

Note that two other sediment fractions distinguished by the WFLOW sediment model are not included in this connection, as they are considered of minor relevance for simulating suspended particulate matter and the associated pollution issues:

- sand with mean diameter 0.200 mm
- large aggregates (lagg) with mean diameter 0.500 mm

This choice was made to keep the communication files as small as possible.

3.5 Output

3.5.1 Output items

In all cells the following output is available.

Table 3.8: *Output*

Name in model	Definition	Unit
Emis_Sfw	emission to surface waters	(g/s)
RO2ComSew	runoff from paved areas to mixed sewers	(m^3/s)
WW2ComSew	wastewater to mixed sewers	(m^3/s)
ConcROp	concentration in runoff from paved areas	(g/m^3)
ConcROu	concentration in runoff from unpaved areas	(g/m^3)
ConcWW	concentration in raw wastewater	(g/m^3)
ConcDR	concentration in drainage from soils	(g/m^3)

Except the emissions themselves, these output items are auxiliary, and can for example be used to validate the model.

These output items can be requested in block 9 of the input file, for inclusion in the regular “his” or “map” output file.

3.5.2 Mass balance output

In addition, all mass fluxes can be retrieved from the model. This entails “release” fluxes, specifying the fluxes released from the different sources to the different model compartments. In addition there are “pathway” fluxes that specify fluxes moving along the pathways to a final destination (storage, removal, emission to surface water).

Table 3.9: Mass balance output

Name in model	Definition	Unit
dRelAtmxxx	Release by atmospheric deposition to compartment	(g/d)
dRelA01xxx	Release from source A01 to compartment xxx	(g/d)
dRelB01xxx	Release from source B01 to compartment xxx	(g/d)
ddww2sew	Pathway flux from domestic wastewater to the sewage collection system	(g/d)
ddww2sfw	Pathway flux from domestic wastewater to surface waters (directly)	(g/d)
ddww2soi	Pathway flux from domestic wastewater to the soil system	(g/d)
dpav2sew	Pathway flux from paved areas to combined sewers	(g/d)
dpav2stw	Pathway flux from paved areas to separated sewers	(g/d)
dpav2sfw	Pathway flux from paved areas to surface waters	(g/d)
dpav2soi	Pathway flux from paved areas to soils	(g/d)
dpav2dec	Pathway flux: decay while on paved areas	(g/d)
dunp2sfwer	Pathway flux from unpaved areas to surface waters by erosion	(g/d)
dunp2sfwro	Pathway flux from unpaved areas to surface waters by runoff	(g/d)
dunp2soiin	Pathway flux from unpaved areas to soils by infiltration	(g/d)
dunp2soibu	Pathway flux from unpaved areas to soils by burial	(g/d)
dunp2dec	Pathway flux: decay while on unpaved areas	(g/d)
dsew2sfwl	Pathway flux from combined sewers systems to surface waters by leakage/CSOs	(g/d)
dsew2rem	Pathway flux: removal (by treatment) from combined sewer systems	(g/d)
dsew2sfwe	Pathway flux from to	(g/d)
dsew2soi	Pathway flux from combined sewers systems to surface waters by WWTP effluents	(g/d)
dsew2sfwu	Pathway flux from combined sewers systems to surface waters by unconnected sewer systems (no WWTP in place)	(g/d)
dstw2rem	Pathway flux: removal from separated sewer systems	(g/d)
dstw2sfw	Pathway flux from separated sewer systems to surface waters	(g/d)
dstw2soi	Pathway flux from separated sewer systems to soils	(g/d)

Table 3.10: *Mass balance output (continued)*

Name in model	Definition	Unit
dsoi2sfwex	Pathway flux from soils to surface waters (exfiltration)	(g/d)
dsop2sfwex	Pathway flux from soils to surface waters (exfiltration; passive pool)	(g/d)
dsoi2rem	Pathway flux: removal in soils	(g/d)
dsoi2sfwer	Pathway flux from soils to surface waters (erosion)	(g/d)
dsop2sfwer	Pathway flux from soils to surface waters (erosion; passive pool)	(g/d)
dsoi2sop	Immobilization flux	(g/d)
dsfw2exp	Emissions to surface waters	(g/d)
dtransfw	Horizontal transport in surface water compartment (inflow minus outflow), only land cells have outflow, outflow from a river cell is the calculated emission	(g/d)
dtransoi	Horizontal transport in soils	(g/d)
dtransop	Horizontal transport in soils (passive pool)	(g/d)

These fluxes will be included in the balance output files ("_bal.his" and "_bal.prn"). They will be located under the relevant compartments, for example:

- ◇ A release flux to the "pav" compartment will be visible in this compartment only and not in the others.
- ◇ A pathway flux from "pav" to "sfw" will be visible in those two compartments and not in the others.

These fluxes allow the user to trace the fate of every gram of matter released in any of the compartments. The "_bal.prn" file provides totals over the whole output period; the "_bal.his" file provides time dependent fluxes.

3.5.3 Example of a mass balance; storage

An example is provided in the box below. This example illustrates how storage appears in the mass balances.

```
Substance Pav                    Sources/Inflows  Sinks/Outflows
-------------------------------------------------------------
Pav   _Storage                      0.00000E+00   -0.93737E+09
Pav   _dRelAtmPav                   0.48006E+10    0.00000E+00
Pav   _dRelA01Pav                   0.00000E+00    0.00000E+00
Pav   _dRelB01Pav                   0.00000E+00    0.00000E+00
Pav   _dpav2sew                     0.00000E+00   -0.13129E+10
Pav   _dpav2stw                     0.00000E+00   -0.10056E+10
Pav   _dpav2sfw                     0.00000E+00   -0.29535E+07
Pav   _dpav2soi                     0.00000E+00   -0.15427E+10
Pav   _dpav2dec                     0.00000E+00    0.00000E+00
SUM OF ALL TERMS                    0.48006E+10   -0.48015E+10
```

This example shows the balance of the paved compartment. The modelled substance is released by atmospheric deposition, and is washed off to various downstream compartments: “sew”, “stw”, “sfw” and “soi”. A part remains on the paved surfaces, shown here as a negative “_Storage” term. This term balances the total of sources and the remaining sinks.

Note that lines with zero values have been omitted for readability.

3.5.4 Example of a mass balance; horizontal transport in the surface waters

Mass balances are made for “land” cells and “river” cells separately, as well as for the sum of all cells. The below example illustrates how horizontal transport is shown in the mass balances.

A technical note: horizontal transport is implemented numerically as a sink in the upstream cell and a source in the downstream cell. The DELWAQ computational framework would also allow the implementation as a transport between cells. In practice, this last option is a lot slower, which is why it was not used. Consequently, the transport related terms in the mass balance are always zero:

```
Sfw   _Other                          0.00000E+00    0.00000E+00
Sfw   _land                           0.00000E+00    0.00000E+00
Sfw   _river                          0.00000E+00    0.00000E+00

============================================================
Mass balances for land
============================================================
Substance Sfw                      Sources/Inflows Sinks/Outflows
------------------------------------------------------------
Sfw   _Storage                        0.00000E+00   -0.10495E+11
Sfw   _dRelAtmSfw                     0.29061E+09    0.00000E+00
Sfw   _dRelB01Sfw                     0.13956E+09    0.00000E+00
Sfw   _dpav2sfw                       0.29535E+07    0.00000E+00
Sfw   _dunp2sfwro                     0.96011E+10    0.00000E+00
Sfw   _dsew2sfwl                      0.75473E+10    0.00000E+00
Sfw   _dsew2sfwe                      0.43886E+11    0.00000E+00
Sfw   _dsew2sfwu                      0.28067E+11    0.00000E+00
Sfw   _dstw2sfw                       0.70389E+09    0.00000E+00
Sfw   _dsoi2sfwex                     0.11054E+09    0.00000E+00
Sfw   _dsop2sfwex                     0.26173E+10    0.00000E+00
Sfw   _dsfw2exp                       0.00000E+00   -0.97471E+07
Sfw   _dtransfw                       0.00000E+00   [-0.82458E+11]
SUM OF ALL TERMS                      0.92965E+11   -0.92963E+11

============================================================
Mass balances for river
============================================================
Substance Sfw                      Sources/Inflows Sinks/Outflows
------------------------------------------------------------
Sfw   _Storage                        0.00000E+00   -0.21303E+02
Sfw   _dRelAtmSfw                     0.86426E+09    0.00000E+00
Sfw   _dRelB01Sfw                     0.48454E+09    0.00000E+00
Sfw   _dpav2sfw                       0.89295E+07    0.00000E+00
Sfw   _dunp2sfwer                     0.00000E+00    0.00000E+00
Sfw   _dunp2sfwro                     0.54627E+10    0.00000E+00
Sfw   _dsew2sfwl                      0.53432E+10    0.00000E+00
Sfw   _dsew2sfwe                      0.27672E+11    0.00000E+00
Sfw   _dsew2sfwu                      0.17437E+11    0.00000E+00
Sfw   _dstw2sfw                       0.52239E+09    0.00000E+00
Sfw   _dsoi2sfwex                     0.16323E+10    0.00000E+00
Sfw   _dsop2sfwex                     0.39342E+11    0.00000E+00
Sfw   _dsoi2sfwer                     0.32040E+11    0.00000E+00
```

```
Sfw   _dsop2sfwer                0.28480E+10    0.00000E+00
Sfw   _dsfw2exp                  0.00000E+00   -0.21612E+12
Sfw   _dtransfw                  [0.82462E+11]    0.00000E+00
SUM OF ALL TERMS                 0.21612E+12   -0.21612E+12
```

For both land and river cells, surface waters receive the modelled substance from atmospheric deposition, from source B01 and from a variety of pathways. The land cells show no (almost) emission to surface water (_dsfw2exp). The sink side of the balance consists mostly of horizontal transport (_dtransfw). This flux arrives in the river cells (in the example), from where it is further processed as an emission (_dsfw2exp). Note that in the overall balance (not shown here), the term _dtransfw disappears.

Note that lines with zero values have been omitted for readability.

3.6 Supporting processes: soil initialization

For modelling certain pollutants, e.g. nutrients, legacy pollutants, it may be required to initialize the soil compartment. This can be done by providing the masses per cell in Section 8 of the input file.

An alternative is to use a supporting process that provides this initialization based on a prescribed soil quality. For nitrogen and phosphorus, such information can be derived from global maps using two additional supportive processes (see Appendix D).

3.6.1 Soil initialization using top soil quality: InitSoi

This process uses a spatial input field specifying the quality of the Soi compartment to initialize the Soi compartment in the first simulation step. The initialization is done by a flux during the first time step, so it will be added to any other initialization for example by a restart.

In addition, the process calculates the quality of the top soil during the simulation as affected by D-Emissions processing.

The process input:

Table 3.11: *Top soil quality*

Name in model	Definition	Unit	Spatial function?	Time dependent?
fUnpaved	fraction unpaved	(-)		No
SoilThick	soil thickness	(mm)		No
SoilPoros	soil porosity	(-)		No
RhoDM	soil dry matter density	(kg/m^3)		No
QTopSoil	concentration of top soil (start of simulation)	(mg/kg)		No
TotArea	total surface area	(m^2)		No
FracPass	fraction to be allocated to passive pool	(-)		No
Soi	mass	(g)		No
SoilPass	mass in passive soil pool	(g)		No

The process output:

Table 3.12: *Top soil quality model: Process output*

Name in model	Definition	Unit
QSoiTot	Simulated concentration of top soil	(mg/kg)

The fluxes output:

Table 3.13: *Top soil quality model: Flux output*

Name in model	Definition	Unit
dInitSoi	Initialization flux for Soi compartment	(g/d)
dInitSoiP	Initialization flux for passive soil store	(g/d)

3.6.2 Directions for use

- ◇ Process *InitSoi* can be used for all pollutants, based on the user-defined quality of the soil *QTopSoil*.
- ◇ For nitrogen and phosphorus respectively, the processes *Soil_Nit* and *Soil_Pho* can be used to provide *QTopSoil*.
- ◇ When using soil initialization, the mass balance for the Soi compartment will show a large initialization flux and an equally large storage flux of opposite sign. These two fluxes probably overshadow all others by many orders of magnitude. This can be avoided by re-setting the output period to start at least one time step after the start of the simulation. In that case the initialization will no longer show in the mass balances.
- ◇ For obvious reasons, the Process *InitSoi* should not be used in a restarted run.

3.7 Other supporting processes

Expert users can add additional supporting processes using the so-called open Processes Library functionality (refer to https://content.oss.deltares.nl/delft3d4/D-Water_Quality_Open_Proc_Lib_User_Manual.pdf of the D-Water Quality software).

Such options are typically used to perform simple calculations to convert the available input maps to the input requirements of the D-Emissions software. This is an alternative to performing these operations in a GIS environment and providing new input maps. The processes textitSoil_Nit and *Soil_Pho* discussed above present relevant examples.

Another typical application is to set transport and fate related parameters dependent of for example soil properties and weather conditions.

The available processes are discussed in Appendix D.

4 Use of D-Emissions

4.1 General

D-Emissions has been set up as an application of the D-Water Quality module (a.k.a. DELWAQ). This means that the available documentation of D-Water Quality provides an exhaustive discussion of input and output options.

Note: the modelled compartments (section 3.2) are represented by D-Water Quality substances. This implies that transports between compartments are represented by D-Water Quality processes that consume one substance (compartment) and produce another substance (compartment).

Note: the D-Water Quality module is mass based, and uses the volumes of the computational elements to calculate substance concentrations. D-Emissions is completely mass based. All volumes are set to 1.0, so what is called “concentration” in the D-Water Quality software is again a mass in D-Emissions.

4.2 Model input file

The D-Emissions input file holds all the input data and input parameters that belong to the emission model. This file satisfies the format requirements of the so-called “D-Water Quality Input File”, as documented in the related manual (https://content.oss.deltares.nl/delft3d/manuals/D-Water_Quality_Input_File_Description.pdf)

The input file must end in “.inp”, but can otherwise have any name. In this chapter, it will be called “runname.inp”.

The most relevant conventions in this input file are:

- ◇ all text that follows a semicolon “;” is considered comment text and will be neglected;
- ◇ all information items, like keywords or numbers, can be freely positioned, but should be separated by blanks or tabs;
- ◇ it is always possible to continue on a new line.
- ◇ at any point in the input file, the keyword “INCLUDE” can be used followed by the name of a text file (“include file”) to embed the contents of that file into the D-Emissions input file. For D-Emissions, this feature is used to embed case-specific information provided by the underlying hydrology model into the input file.

The input file is divided in 10 sections, each of them ending with ‘#1’, ‘#2’, etc. up to ‘#10’. An input file template is available. This template refers to so-called “include files” that are prepared by an underlying hydrology model and that provide schematization, land use data and hydrology data.

Table 4.1: *Input sections*

Section	Contents	In D-Emissions ...
1	identification, substance IDs	Generic template, with case specific include files from the WFLOW coupling (config B1_xxx)
2	Simulation timers, output times and locations	Generic template, with case specific include files from the WFLOW coupling B2_xxx)
3	Model grid	Generic template, with case specific include files from the WFLOW coupling (B3_xxx)
4	Transport definitions	Generic template, D-Emissions does not use this functionality
5	Open boundary conditions	Generic template, D-Emissions does not use this functionality
6	Waste loads	Generic template, D-Emissions does not use this functionality
7	Process steering	Generic template holds obligatory input items, user to provide D-Emissions key input, see also Section 4.3
8	initial conditions	Generic template, optional restarting, see Section 4.6
9	output specification	Generic template, optional user defined selection of output, see Section 4.5.2
10	statistical output	Empty by default, optional definition of statistic output, see Section 4.5.5

Primarily, the user has to complete section 7 of the input file following the guidance provided in this manual. Here two types of input items can be provided.

Constant values, for example model parameters, are provided as follows:

```
CONSTANTS name DATA number
```

Names of input items are provided in Section 3.4. Numbers to specify values are obviously the user's responsibility.

Spatial data are provided as follows (using text files):

```
PARAMETERS name ALL DATA INCLUDE myfile   ; if myfile is a text file
```

Where "myfile" is a reference to a file name that holds the spatial data File names need to have absolute or relative (to run directory) paths included. Embedded blanks are only allowed if the path and file are included in single quotes[9].

Spatial data are provided in text format as a list of numbers for all schematization elements in the proper order. For WFLOW applications this is the "DN" number.

Alternatively, spatial data are provided in a binary format by WFLOW:

```
PARAMETERS name ALL BINARY_FILE myfile   ; if myfile is a binary file
```

4.3 Coupling to WFLOW hydrology and sediment models

D-Emissions can use the following input items provided by the coupling to WFLOW (hydrology and sediment). The table indicates whether the use of these items is compulsory.

Table 4.2: *Input sections for coupling with WFLOW*

Item name	File name	Keyword to use	Compulsory
TotArea	B7_geometry.inc[10]	PARAMETERS	Yes
fPaved	B7_geometry.inc	PARAMETERS	Yes
fUnpaved	B7_geometry.inc	PARAMETERS	Yes
fOpenWater	B7_geometry.inc	PARAMETERS	Yes
River	staticdata\river.dat	PARAMETERS	Yes
Downstream	staticdata\ptiddown.dat	PARAMETERS	Yes
Rainfall	B7_hydrology.inc and dynamicdata\hydrology.bin	SEG_FUNCTIONS	Yes
RunoffPav	B7_hydrology.inc and dynamicdata\hydrology.bin	SEG_FUNCTIONS	Yes
RunoffUnp	B7_hydrology.inc and dynamicdata\hydrology.bin	SEG_FUNCTIONS	Yes
Infiltr	B7_hydrology.inc and dynamicdata\hydrology.bin	SEG_FUNCTIONS	Yes
Exfilt	B7_hydrology.inc and dynamicdata\hydrology.bin	SEG_FUNCTIONS	Yes
Subsurface	B7_hydrology.inc and dynamicdata\hydrology.bin	SEG_FUNCTIONS	Yes
Overland	B7_hydrology.inc and dynamicdata\hydrology.bin	SEG_FUNCTIONS	Yes
ErodIM1	B7_sediment.inc and dynamicdata\sediment.dat	SEG_FUNCTIONS	No
ErodIM2	B7_sediment.inc and dynamicdata\sediment.dat	SEG_FUNCTIONS	No
ErodIM3	B7_sediment.inc and dynamicdata\sediment.dat	SEG_FUNCTIONS	No
Tempair	B7_climate.inc and dynamicdata\climate.dat	SEG_FUNCTIONS	No
SoilThick	staticdata\soilthickness.dat	PARAMETERS	Yes
SoilPoros	staticdata\porosity.dat	PARAMETERS	Yes

[9]) Used during model initialization to derive the fate of wastewater. File names need to have

absolute or relative (to run directory) paths included. Embedded blanks are only allowed if the path and file are included in single quotes.

[10]) Used during model initialization to derive the fate of wastewater. The coupling also provides an alternative format using a (more compact) binary data file; B7_geometry-parameters.inc and B7_geometry.bin.

Note that the item “Tempair” is not used by the main D-Emissions process, but is optionally required by supportive processes.

4.4 Running D-Emissions

As all D-Water Quality simulations, running D-Emissions proceeds in two steps. These steps use standard software, enhanced with a so-called OpenPB plugin that holds the D-Emissions formulas.

This plug-in consists of:

- ◇ D3Dwaq_OpenPL.dll
- ◇ A couple of files with names proc_def.dat and proc_def.def

The running commands (Windows OS) for both steps are:

```
..\programs\delwaq\bin\delwaq1.exe espace.inp
                -p  ..\programs\EM-Plugin\Tables\proc_def

..\programs\delwaq\bin\delwaq2.exe espace.inp
                -openpb  ..\programs\EM-Plugin\x64\Release\D3Dwaq_OpenPL.dll
```

Note that the <runname> is “espace” in this example.

Note that these commands include paths for the standard delwaq1 and delwaq2 executables and for the definition of the plugin files. These need to be modified dependent on how the user organizes the programs.

Errors during step 1 are probably caused by typo’s in the <runname>.inp file. See the guidance in the section above to check your edits. This should normally be enough to find the problem. The <runname>.lst file contains a report of the errors. Interpretation of this file requires some familiarity to the D-Water Quality Input File format.

If step 1 was successful, step 2 usually does not produce errors. A window appears that scrolls through the calculation steps until the end of the simulation:

4.5 Output

The model creates the following output files:

- ◇ <runname>.lst: input file report, provides information on input errors;
- ◇ <runname>.lsp: input file report, provides information on use of input data and parameters;
- ◇ <runname>.his: model-wide account of substance content of the model compartments (in g) as they vary over time;

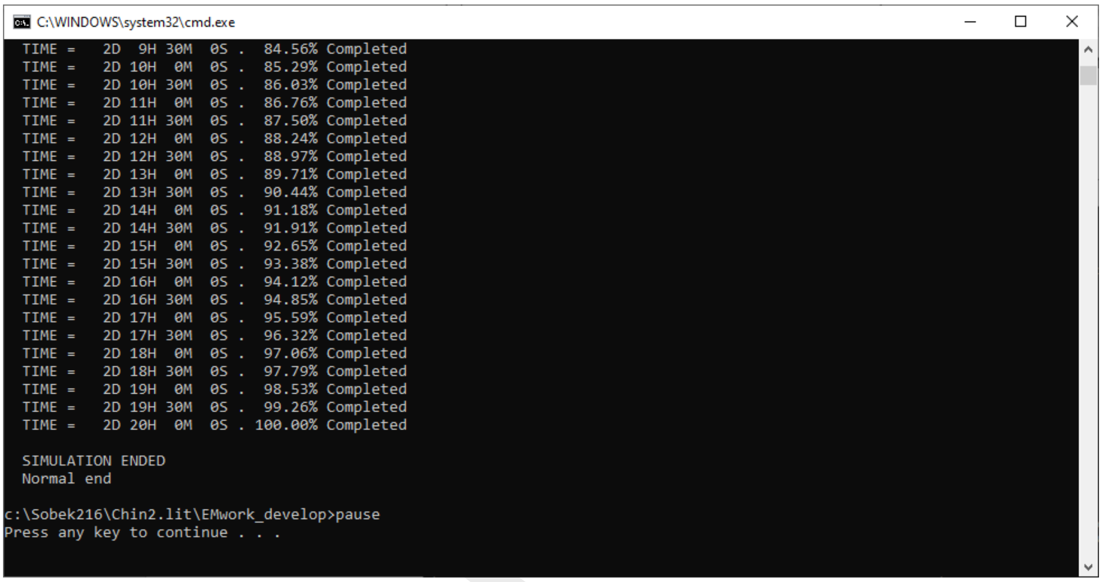

Figure 4.1: *Example of simulation screen*

- <runname>-bal.his: model-wide flux-based outputs (g/putput interval) for the model compartments as they vary over time;
- <runname>.prn: tabulated cumulative fluxes (g/total run period) for the model compartments;
- <runname>.map: spatial and time dependent output data (available for any of the quantities mentioned in section 3);
- <runname>-stat.map: spatial statistics of output data (available for any of the quantities mentioned in section 3).

The definition of the output follows common D-Water Quality practices. This will be briefly explained in the sections below. For details, reference is made to the D-Water Quality input file description.

4.5.1 Output locations

The default files written by WFLOW that define the output locations comprise:

- Any monitoring points set in WFLOW (config\B2_stations.inc)
- Two monitoring areas, one comprising all land cells and one comprising all river cells.

History output will include stations and monitoring areas. Mass balance output will always include monitoring areas and stations only if the keyword "NO_BALANCE" is omitted in their definition:

```
StationA              1    1423
        ; station in DN = 1423, will be included in balances
StationB  NO_BALANCE 1    2781
        ; station not included in balances
```

Map files by definition contain values for all cells.

4.5.2 Additional output variables

The template file defines all compartments masses (g) as history output and no map output. In Section 9 of the file, additional output may be defined. An example:

```
; Ninth input block
 1                                ; Conditions follow in this file
 1                                ; Monitor-file
 0                                ; Grid-file
 2                                ; His-file; all pools + user defined output
 1                                ; count of user defined output
QSoiTot   Volume
 3                                ; only user defined output
 1                                ; count of user defined output
QSoiTot
```

In this example, the output item QSoiTot is added to both the his and the map output. Note that a second item, in this case the word "Volume", is used while defining his output. This is obligatory to determine the averaging algorithm for monitoring areas consisting of more than one cell. The word "Volume" indicates volume-weighing. An empty string (embedded in single quotes), indicates no averaging. For map output, this is irrelevant.

Any input or output item of any process can be requested as output.

4.5.3 Output timers

Output timers are derived from an include file by default (Section 2):

```
INCLUDE 'config\B2_outputtimes.inc'
```

This include file can be disabled by the comment character ";" and replaced by its contents, modified as appropriate. The below example shows how the first day is omitted from the mass balance output:

```
;INCLUDE 'config\B2_outputtimes.inc'
  2010/01/04-00:00:00  2020/12/31-00:00:00  001000000 ; mon/bal
  2010/01/03-00:00:00  2020/12/31-00:00:00  001000000 ; map
  2010/01/03-00:00:00  2020/12/31-00:00:00  001000000 ; his
```

4.5.4 Tailoring mass balances

D-Water Quality offers some keywords in Section 2 to tailor the mass balances output. These keywords are included in the template. There is a separate manual dedicated to this form of output and th tailoring using these keywords (https://content.oss.deltares.nl/delft3dfm2d3d/D-Water_Quality_Mass_Balances.pdf).

4.5.5 Statistical output

D-Water Quality offers functionality to provide statistical output. This is requested in Section 10, and explained in Appendix D of the related User Manual (https://content.oss.deltares.nl/delft3dfm2d3d/D-Water_Quality_User_Manual.pdf). The below provides an example:

```
period 'y11'
   suffix     'y11'
```

```
   start-time '2011/01/01-00:00:00'
   stop-time  '2012/01/01-00:00:00'
end-period

output-operation 'STADSC'
   substance 'Emis_Sfw'
   suffix    ''
end-output-operation
```

This example will write the min, mean and max values of the emissions to surface water over the year 2011 into the <runname>-stat.map file.

4.6 Restarting D-Emissions

Restarting is arranged in Section 8. The below shows how the default initialization is disabled by the ";" comment character and a restart file from a previous run is used. Note that this restart file was written by a run using input file EMNitSU.inp.

```
;INITIALS  Sew Pav Unp Stw Sfw Soi
;DEFAULTS  6*0.0
'EMNitSU_res.map'
```

4.7 Coupling to D-Emissions to a river water quality (WQ) model

This section is not intended to cover all aspects of setting up a water quality model. Only those aspects specific for linking a water quality model to WFLOW and a WFLOW based D-Emissions model are discussed here.

It is noted that the WFLOW based water quality model operates for WFLOW river cells only. WFLOW land cells are part of the D-Emissions schematization. The emissions are routed in D-Emissions to the river cells, and written as output for input in the water quality model.

The coupling to WFLOW entails four transport fluxes for each river cell:

1. The outflow to the downstream cell, or to the outflow point(s) of the model, indicated by "sfw>out"
2. The inflow from surface runoff, indicated by "land>sfw"
3. The subsurface inflow, indicated by "soil>sfw"
4. A vertical flux that can be used for particle modelling, to represent the settling process, indicated by "sfw>sett"

4.7.1 WQ model derived from WFLOW

The D-Water Quality input file holds all the input data and input parameters that belong to the water quality model. This file satisfies the format requirements as documented in the related manual (https://content.oss.deltares.nl/delft3d/manuals/D-Water_Quality_Input_File_Description.pdf).

At any point in the input file, the keyword "INCLUDE" can be used followed by the name of a text file ("include file") to embed the contents of that file into the D-Water Quality input file. This feature is used to embed case-specific information provided by the underlying hydrology model into the input file. An input file template is available to demonstrate this.

Table 4.3: Input sections with WFLOW

Section	Contents	In D-Emissions ...
1	identification, substance IDs	Generic template, with case specific include files from the WFLOW coupling (config B1_xxx), WQ model specific input to be added
2	Simulation timers, output times and locations	Generic template, with case specific include files from the WFLOW coupling B2_xxx)
3	Model grid	Generic template, with case specific include files from the WFLOW coupling (B3_xxx and dynamic-data\volume.dat)
4	Transport definitions	Generic template, with case specific include files from the WFLOW coupling (config\B4_xxx and dynamic-data\flow.dat)
5	Open boundary conditions	Generic template, with case specific include files from the WFLOW coupling (config\B5_xxx)
6	Waste loads	Generic template, D-Emissions does not use this functionality
7	Process steering	Generic template holds obligatory input items, plus standard process to couple to D-Emissions and to provide basic hydraulics (see following sections), WQ model specific input to be added
8	initial conditions	Generic template, optional restarting, WQ model specific input to be added
9	output specification	Generic template, optional user defined selection of output, see Section 4.5.2, WQ model specific input to be added
10	statistical output	Empty by default, optional definition of statistic output, see Section 4.5.5

In the table above, “WQ specific input” refers to the selection of state variables, processes, initial conditions and extra output items typical for a water quality model. This is the kind of information that is provided by a so-called “sub-file”. However, this subfile needs to be converted manually to a suitable set of include files. This will not be discussed further in this D-Emissions manual. Reference is made to the D-Water Quality documentation.

4.7.2 Linking D-Emissions to the WQ model

The D-Emissions model writes its emission data into two files, always called:

```
outdata_em.bin
outdata_em.txt
```

In the case that multiple D-Emissions model runs are carried out, e.g. for total nitrogen (TN) and total phosphorus (TP), it is up to the user to arrange that these files get substance-specific names or are stored in separate folders, so that it is avoided that the results for TP overwrite those for TN.

D-Water Quality is equipped with processes able to read these files and translate them into the appropriate state variables (e.g. NH4, NO3, PON1 etc. for TN; AAP, PO4, POP1 for TP). This allows D-Water Quality to simulate their fate in the surface water using standard processes from the library.

This series of processes is called EM_xxx. Every individual EM_xxx process is configured to use one `outdata_em.bin` file as a space- and time-dependent forcing function (keyword SEG_FUNCTIONS) in Section 7 of the input file. The details are discussed in the next section.

4.7.3 WQ processes EM_xxx (xx = BOD, TNI, TPH, TSS, COL, TRA)

To activate the relevant process in block 7 of the WQ input file:

```
CONSTANTS Active_EM_xxx DATA 1
```

To connect a E_Emissions output file:

```
SEG_FUNCTIONS EmisWxxx ALL BLOCK BINARY_FILE outdata_em.bin
```

The functionality to distribute the emission data over several state variables (also known as “USEFOR” functionality) is included in the EM_xxx process. Input can be provided by the user in the following way:

```
CONSTANTS xxxtoyyy DATA 0.3
```

In this example xxx is the emission model output variable, yyy is the receiving water quality model state variable, and 0.3 is the fraction of xxx allocated to yyy.

The table below lists the available options for xxx, and the equivalent definitions.

Table 4.4: *Available input options*

xxx	WQ process	Item name for total emissions	Item names for scaling factors	Calculated fluxes
BOD	EM_BOD	EmisWBOD	n.a. (all emissions to CBODu)	dEBODu
TNI	EM_TNI	EmisWTNI	TNItoNH4, TNItoNO3, TNItoPON1, TNItoPON2, TNItoDON	dENH4, dENO3, dEPON1, dEPON2, dEDON
TPH	EM_TPH	EmisWTPH	TPHtoPO4, TPHtoAAP, TPHtoPOP1, TPHtoPOP2, TPHtoDOP	dEPO4, dEAAP, dEPOP1, dEPOP2, dEDOP
TSS	EM_TSS	EmisWTSS	TSStoIM1, TSStoIM2, TSStoIM3	dEIM1, dEIM2, dEIM3
COL	EM_COL	EmisWCOL	COLtoEColi, COLtoFColi, COLtoTColi	dEEColi, dEFColi, dETColi
TRA	EM_TRA	EmisWTRA	TRAtocTR1, TRAtodTR1, TRAtocTR2, TRAtodTR2	dEcTR1, dEdTR1, dEcTR2, dEdTR2

So, for illustration, to set up a model for nitrogen and phosphorus, the user has to provide in the WQ model input file:

```
CONSTANTS Active_EM_TNI DATA 1
SEG_FUNCTIONS EmisWTNI ALL BLOCK BINARY_FILE ..\EM_NIT\outdata_em.bin

CONSTANTS TNItoNH4 DATA 0.2
CONSTANTS TNItoNO3 DATA 0.4
CONSTANTS TNItoPON1 DATA 0.4

CONSTANTS Active_EM_TPH DATA 1
SEG_FUNCTIONS EmisWTPH ALL BLOCK BINARY_FILE ..\EM_PHO\outdata_em.bin

CONSTANTS TPHtoPO4 DATA 0.5
CONSTANTS TPHtoAAP DATA 0.4
CONSTANTS TPHtoPOP1 DATA 0.1
```

4.7.4 WQ process WFLOW_Hydr

This process is available in D-Water Quality to provide some hydraulic properties that the WFLOW coupling does not provide, in particular the velocity, the depth and the shear stress.

The process input:

Table 4.5: *Available input options*

Item name	Description	Unit	Provided by
Volume	volume of segment	(m^3)	WFLOW
Surf	horizontal surface area of segment	(m^2)	WFLOW
Riverlen	river length in segment	(m)	WFLOW
Chezy	Chezy coefficient	($\sqrt{m}$/s)	user
Flow	Outflow from segment	(m^3/s)	WFLOW

It is noted that the river length in WFLOW is often derived from a real river trajectory map. The length is therefore not by definition equal to one of the sides or the diagonal of a grid cell. This is consistently processed also for the volume and horizontal surface area.

The process output:

Table 4.6: *Available output options*

Item name	Description	Unit
Velocity	horizontal flow velocity	(m/s)
Depth	depth of segment	(m)
TotalDepth	depth of column (equal to depth)	(m)
Tau	total bottom shear stress	(N/m^2)

4.8 Plotting map output

4.8.1 Using UGRID compliant NetCDF files

D-Emissions and D-Water Quality, when linked to WFLOW, are planned to have output in UGRID compliant NetCDF files. This file format includes the spatial (unstructured) grid information, so could be used for plotting maps without additional information.

For both D-Emissions and D-Water Quality this requires:

- ◇ The inclusion of an include file providing the UGRID formatted grid information in the input file, at the top of Section 3:

```
UGRID 'config\B3_waqgeom.nc'
```

- ◇ The activation of NetCDF map output in Section 9:

```
; formats of History/Map
1                          1        ; switch on  binary History file
0                              0        ; switch off binary Map     file
0                              0        ; not used
1                              1        ; switch on  NetCDF Map     file
```

These NetCDF map files can be directly postprocessed using Quickplot or QGIS.

4.8.2 Using traditional output

The binary map file output files of D-Emissions and D-Water Quality, the time dependent normal map file and the statistics map file, can not be directly plotted as maps since they do not contain spatial grid information.

A Managing the proc_def files

A.1 General

This appendix is only intended for expert users and for the maintenance team.

Part of the implementation of D-Emissions in Delft3D-Water Quality is provided in the form of the proc_def.dat and proc_def.def files (Section 4.4). These files are a binary representation of a collection of comma-separated-value files that comprise the administration of the Processes Library. To generate these files, two steps are needed, as outlined below.

A.1.1 Generating a text file version (proces.asc)

The developers of D-Emissions create a so-called “proces.asc” file, which is a text file version of proc_def. This text file version is initially created for 1 type A source and 1 type B source (Section 3.3.1). A dedicated tool, GenerateTables.exe, is able to adapt this file for multiple sources of both types.

The tool is operated from a command prompt:

```
GenerateTables.exe proces11.asc proces.asc 1 3 12 2 7 63 31 nowwman
```

There are the following command line arguments:

1 The input proces.asc file for 1 type A source and 1 type B source
2 The output proces.asc file
3 The desired number of Type A sources
4 The number of variables to describe a Type A source (3 in current version)
5 The desired number of Type B sources
6 The number of variables to describe a Type B source (2 in current version)
7 The receptor count (exclusive of SoilPass) (7 in current version)
8 The number of input items preceding the input items for the sources (63 in the current version)
9 The number of pathway-related fluxes (31 in the current version)
10 A keyword “wwman” or “nowwman”, indicating if the GenWWMan process exists (does not exist anymore in the current version, so “nowwman” is to be used). Note: Most of these arguments are fixed for a given version of D-Emissions. They allow the use of the same tool also for older versions.

A.1.2 Generating the binary proc_def files

To further process the proces.asc file as discussed above, two standard Delft3D tools are used, as in the below scheme.

- The standard tool waqpb_import creates a collection of csv-files, that comprise the administration of the Processes Library derived from the proces.asc file.
- The standard tool waqpb_export creates the proc_def tables needed for a simulation with D-Emissions.
- That tool also creates a procesm.asc file, that is supposed to be a mirror of the original proces.asc file. It is used to verify that the process has been executed correctly.

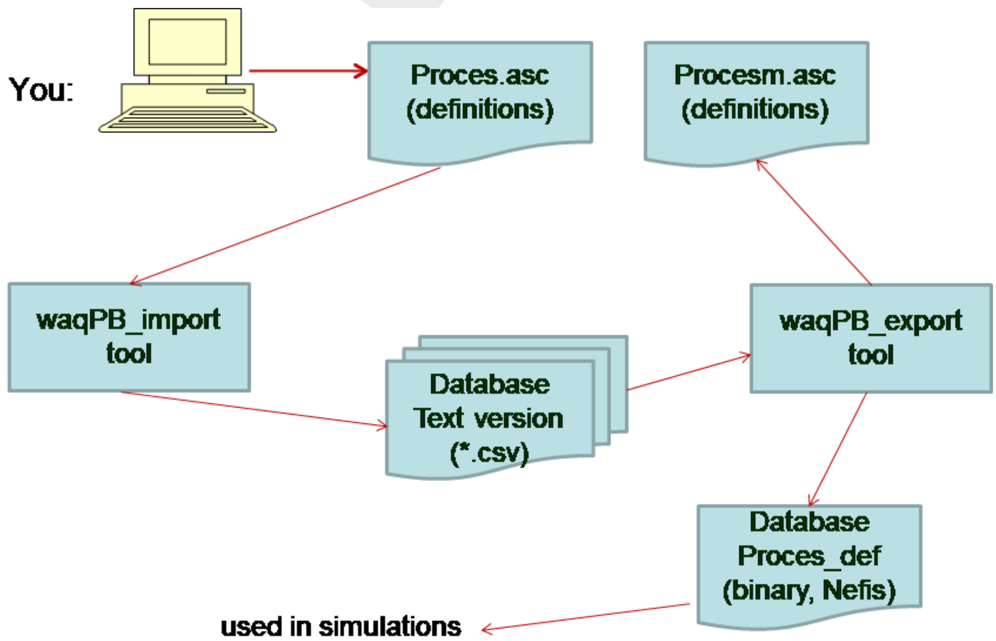

Figure A.1: *Example of simulation screen*

B Changes relative to older versions

B.1 Relative to version released in June 2022

Main differences are:

- Different way of dealing with the soil compartment;
- Integration of GenWWMan process (supportive process to calculate fate of wastewater and overall treatment efficacy;
- Introduction of Domestic wastewater as a separate compartment;
- Introduction of sediment fluxes to drive erosion process;
- Some previously hardcoded parameters are now available as input;
- The share of wastewater and the share of stormwater intercepted by sewer systems can now be defined separately;
- Additional output from EM for validation purposes;
- Separation in output of certain fluxes between compartments;
- The “kd” parameters are now defined as the dissolved fraction (not the fraction in the solid phase);
- Different definition of the water quality model, on river cells only, which implies that EM deals with horizontal transports between land cells;
- Soil thickness now defined in mm and not in m.

To be implemented:

- Different definition of horizontal transfers of water in Sew and Stw.

B.2 Guidance for update of input files

B.2.1 EM

Ascertain that the input file is consistent with the template input file

- Add a state variable “Dww”.
- Replace state variable SoilStore by SoilPass (new Soil approach);
- Connect to WFLOW using the latest WFLOW coupling ;
- Include River and Downstream items in Section 7 using WFLOW data (see template);
- Include SoilThick and SoilPoros in Section 7 using WFLOW data (see template);
- Note the change of the unit of Soilthick (currently mm).

Update user input

- Redefine parameters KdUnpa (dissolved fraction, no longer fraction in solid phase);
- Define KdSoi, ImmoSoi, CBack (new Soil approach);
- Define FrRainSew (new parameter, previously same as FrSewered);
- If you weren’t using the supporting wastewater management process (GenWWMan), replace the input parameters Eff_WWTP and Sld_WWTP by the parameters listed in this manual under wastewater management.

B.2.2 WQ

Ascertain that the input file is consistent with the template input file.

C Some additional processes for WFLOW-based water quality modelling

These processes are not directly linked to D-Emissions, so they are not included in the main body of this report.

C.1 Coupling a water quality model to the sediment delivery to streams

Process: **SEDIMLINK**

WFLOW has a sediment module that can perform a full sediment calculation by itself. It is however also possible to pick up the sediment delivered to river cells calculated by WFLOW in a water quality model. This requires:

- Including the creation of the sediment model output in the WQ coupling of WFLOW.
- Using the SEDIMLINK process to include the sediment delivered to river cells as a source of sediments in the DELWAQ model.

The process input:

Table C.1: *Process input*

Item name	**Description**	**Unit**
ErodIM1-6	Sediment delivery of fractions 1-6	(g/d)
FacErod	Scale factor to be applied to the sediment delivery	(-)

The process output:

Table C.2: *Process output*

Item name	**Description**	**Unit**
TotErod	Sum of sediment delivery for fractions 1-6	(g/d)

The fluxes output:

Table C.3: *Fluxes output*

Item name	**Description**	**Unit**
dErSus1-6	Flux of IM1-6 added to the model	(g/m)

Directions for use:

- Typically, only the finer fractions 1-3 are actually used. The coarser fcations are not transported in suspension, and therefore have limited relevance for the water quality.
- The template input file contains an example of how the out from WFLOW is embedded in the WQ model.

C.2 Define temperature of inflowing water

Process: **TempDifInf**

Using atmospheric forcing data provided by the WFLOW coupling, a river water temperature model can be defined, using standard functionality to simulate the heat exchange between surface water and the atmosphere. This auxiliary process allows the definition of the temperature of the water flowing into the river network, again based on information provided by by the WFLOW coupling. This requires:

- ◇ Including the creation of the atmospheric meteo forcing in the WQ coupling of WFLOW.
- ◇ Using the TempDifInf process to set the temperature of the inflowing water.

The process input:

Table C.4: *Process input*

Item name	Description	Unit
TempAir	Air temperature	degC
AvPerDifT1	Averaging period for temperature of surface runoff	d
AvPerDifT2	Averaging period for temperature of subsurface inflow	d
TemMin	Minimum temperature of runoff	degC

The fluxes output:

Table C.5: *Process output*

Item name	Description	Unit
dDifTemp	Influx of heat by surface runoff and subsurface flow	degC/m^3/d

Directions for use:

- ◇ The averaging period for surface runoff is typically set to a small value, while the averaging period for subsurface inflows is set to a higher value. This is done to reflect the damping of temperature fluctuations in the subsoil.
- ◇ The minimum temperature prevents the inflow of water below a certain temperature. Obviously, this value is typically 0 or a little higher.

D Supportive processes

D.1 Nitrogen in top soils: process Soil_Nit

This process is tailored to the data available from:
https://doi.org/10.17027/isric-soilgrids/d95b6733-5a29-475e-ab83-478dcb8c0c20.

This data source provides total nitrogen in cg/kg at 6 standard depths at a 1000m resolution. After projection on the WFLOW grid by the user, the process uses data at up to 3 depths and allows the user to set scale values for these three depths. The result is converted to mg/kg.

Note: This can be supported by HydroMT.

The process input:

Table D.1: *Process input*

Item name	Description	Unit	Spatial function	Time dependent
nit_layer1	SoilGrids N content 0-5cm	Cg/kg		No
nit_layer2	SoilGrids N content 5-15cm	Cg/kg		No
nit_layer3	SoilGrids N content 15-30cm	Cg/kg		No
fac_layer1	Scale factor for data from layer 1	-		No
fac_layer2	Scale factor for data from layer 2	-		No
fac_layer3	Scale factor for data from layer 3	-		No

The process output:

Table D.2: *Process output*

Item name	Description	Unit
QTopSoil	concentration of top soil	mg/kg

D.2 Phosphorus in top soils: process Soil_Pho

This process is tailored to the data available from
http://dx.doi.org/10.3334/ORNLDAAC/1223.

This data set provides estimates of different forms of naturally occurring soil phosphorus (P) including labile inorganic P, organic P, occluded P, secondary mineral P, apatite P, and total P on a global scale at 0.5-degree resolution. The unit is g m^{-2} calculated over the top 50 cm of the soil. After projection on the WFLOW grid by the user, the process uses a selected variable of this dataset and converts it to mg/kg.

Note: This can be supported by HydroMT.

The process input:

Table D.3: Process input

Item name	Description	Unit	Spatial function	Time dependent
pho_tot	Input P concentration	g/m^2		No
PDatThick	Layer thickness for input field (default 0.5 m)	m		No
SoilPoros	Soil porosity	-		No
RhoDM	Dry matter density	kg/m^3		No

The process output:

Table D.4: Process output

Item name	Description	Unit
QTopSoil	concentration of top soil	mg/kg

D.3 Atmospheric deposition of nitrogen: process EMEP_Nit

This process is tailored to the data available from the European Monitoring and Evaluation Programme EMEP
https://www.msceast.org/pollution-assessment/emep-domain-menu/data-hm-pop-menu.

This data source provides the wet and dry deposition of reduced and oxidized nitrogen together with the rainfall on a 0.1-degree resolution rectangular grid. This process converts these data in their units as provided by the data source to dry and wet nitrogen deposition rates in the correct units for D_Emissions.

The process input:

Table D.5: Process input

Item name	Description	Unit	Spatial function	Time dependent
DDp_Nox	Dry deposition of oxidised N	$mg/m^2/y^1$		No
DDp_Nred	Dry deposition of reduced N	$mg/m^2/y^1$		No
WDDp_Nox	Dry deposition of oxidised N	$mg/m^2/y$		No
WDp_Nred	Dry deposition of reduced N	$mg/m^2/y$		No
WDp_Rain	Wet deposition, rainfall	mm/y		No

[1]: The input item “scalDum” can be used to scale this input item if it is available in a different unit.

The process output:

Table D.6: *Process output*

Item name	Description	Unit
EF_DDp	Dry deposition rate	g/m^2/d
EF_WDp	Wet deposition rate (concentration in rainfall)	g/m^3
NDepTot	Total deposition (from input)	g/m^2/d

The functional conversions are:

$$EF\_DDp = DDp\_Nox + DDp\_Nred$$
$$EF\_WDp = \frac{WDp\_NOx + WDp\_Nred}{WDp\_Rain}$$
$$NDeptTot = EF_{DDP}\frac{WDp\_NOx + WDp\_Nred}{1000 \times 365}$$

D.4 Temperature dependent fate parameters: process SetFate

This process sets temperature dependent values of 5 transport and fate parameters, all using the generic formula:

$$k(T) = k(T = 20) \times \theta^{(tempair-20)}$$

The process input:

Table D.7: *Process input*

Item name	Description	Unit
DecPav20	decay rate paved at ref temp	(1/d)
DecUnp20	decay rate unpaved at ref temp	(1/d)
DecSoi20	decay rate soils at ref temp	(1/d)
KdUnpa20	fraction of bound vs unbound at ref temp	(-)
KdSoi20	fraction of bound vs unbound at ref temp	(-)
DecPavThet	temp. dependency constant for decay rate paved	(-)
DecUnpThet	temp. dependency constant for decay rate unpaved	(-)
DecSoiThet	temp. dependency constant for decay rate soils	(-)
KdUnpaThet	temp. dependency constant for fraction bound	(-)
KdSoiThet	temp. dependency constant for fraction bound	(-)
Tempair	temperature of top soil	(degC)

[1]: The input item “scalDum” can be used to scale this input item if it is available in a different unit.

The process output:

Table D.8: *Process output*

Item name	Description	Unit
DecPav	decay rate paved	(1/d)
DecUnp	decay rate unpaved	(1/d)
DecSoi	decay rate soils	(1/d)
KdUnpa	fraction of bound vs unbound	(-)
KdSoi	fraction of bound vs unbound	(-)

D.5 Partitioning in soils: process SetSoiKd

This process sets the fraction of the substance in the soil moisture using a partitioning concept:

$$f_{dis} = \frac{1}{1 + K_d(1 - Poros)\rho_{DM}}$$

where f_{dis} is the fraction in soil moisture, K_d is the dry matter partition coefficient in m^3/kg and ρ_{DM} is the density of the solid phase in kg/m^3. The partition coefficient is either read from the input, or calculated from an organic carbon partition coefficient, using the soil organic matter fraction.

The process input:

Table D.9: *Process input*

Item name	Description	Unit
SoilPoros	soil porosity	(-)
RhoDM	soil dry matter density	(kg/m^3)
SoilOM	soil organic matter fraction	(-)
SoilKd	partition coefficient	(m^3/kgDM)
SoilKoc	soil organic carbon part coeff	(log(l/kgOC))

The process output:

Table D.10: *Process output*

Item name	Description	Unit
KdSoi	fraction in soil moisture	(-)

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