Water quality and aquatic ecology modelling suite

D-Water Quality

Deltares systems

Sediment Water Interaction

User Manual

Deltares

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D-Water Quality

Version: 2027.01
Revision: 80917

10 October 2026

Sediment Water Interaction, User Manual

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Published and printed by:
Deltares
Boussinesqweg 1
2629 HV Delft
P.O. 177
2600 MH Delft
The Netherlands

telephone: +31 88 335 82 73
e-mail: Information
www: Deltares

For sales contact:
telephone: +31 88 335 81 88
e-mail: Sales
www: Sales & Support

For support contact:
telephone: +31 88 335 81 00
e-mail: Support
www: Sales & Support

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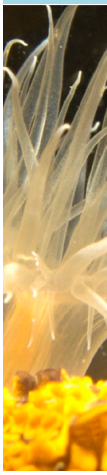
Preface

This additional manual deals with the input for new functionality that is not supported in the user interfaces, in particular the concepts of and the additional input for the modelling of sediment quality and sediment-water interaction. The use of the new functionality requires editing of D-Water Quality's ascii input files. A full description of the D-Water Quality input file can be found in Deltares (2026a). This document describes what to add to these files for multilayer sediment quality and sediment-water interaction.



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1 Introduction

This manual constitutes an addition to the main user manuals for D-Water Quality, which can be used stand-alone but is also included in the modeling suits SOBEK and Delft3D. The main user manuals describe the creation of input via the dedicated graphical user interfaces. The present additional manual deals with the input for new functionalities that are not supported by the user interfaces, in particular for the modelling of sediment quality and sediment-water interaction.

The use of the new functionalities requires editing of D-Water Quality's ascii input files. The information allows the user to edit basic input files that have been created with Delft3D's or SOBEK's user interface. A full description of the input file can be found in Deltares (2026a). It is advisable to start reading this manual first to understand the principles of the input file. A **warning** should be given here: the input file is generally the output file of the GUI. This means that your modifications generally do not enter into the GUI again and any modified ASCII file will generally be overwritten by the GUI if you do not make the precaution to store it in a safe place and/or under a safe name.

chapter 2 of this manual is devoted to sediment-water interaction modeling with D-Water Quality. Consecutively, the modeling concept for sediment-water interaction, the formulations for mass transport in the sediment and the sediment specific input are described.

For other model documentation on the structure, concepts, basic formulations and numerical methods the user is referred to the Deltares (2026c) and Deltares (2026a). The same holds for guidance as to running the model and error messages. Moreover, the description of simulated substances, process formulations, and input and output parameters is not included in this manual. The D-Water Quality user is referred to the Deltares (2026b), for a full account of the contents of D-Water Quality's extensive processes library.

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2 Modelling of sediment-water interaction with D-Water Quality

2.1 Modelling concepts and development status

Originally D-Water Quality contained two alternative options for sediment-water interaction modelling, the so-called S1/S2 approach and the SWITCH module.

The S1/S2 approach concerns simplified modelling: The active sediment layer is not modelled as such, but is represented by one or two sets of settled substances that are decomposed, which leads to return fluxes of nutrients, a consumption flux of oxygen and burial fluxes. The S1/S2 approach is still available and is described in D-Water Quality's Technical Reference Manual.

SWITCH was a rather complex process routine that simulates the vertical concentrations gradients of organic matter, oxygen, nitrate and nutrients (N, P, Si) taking into account 4 sediment layers, and that generates similar fluxes as well as the denitrification flux and the phosphate adsorption and precipitation fluxes. SWITCH was fixed with respect to the substances and layers, and was therefore not generic and not very flexible. SWITCH is no longer available in D-Water Quality.

In 2002 a start was made to extend D-Water Quality with the functionalities and process formulations needed to simulate sediment-water interaction and sediment diagenesis in a generic and comprehensive way. To fully and optimally take into account sediment-water interaction in water quality modelling D-Water Quality now facilitates the simulation of both water layers and sediment layers. The sediment and water quality processes are identical as to substances and kinetic formulations. The process formulations are generic. However, the local chemical conditions such as the dissolved oxygen concentration determine how processes turn out. D-Water Quality has been extended with:

- a computational grid for the active sediment layer (in addition to the computational grid for the overlying water), including a "deep" sediment boundary for the lower sediment layer deep;
- keywords to define this grid in D-Water Quality's input;
- a process routine for vertical mass transport (included in D-Water Quality's processes library), that also delivers the exchange fluxes between sediment and overlying water, and between the lower sediment layer and the "deep" sediment boundary;
- input parameters to define the number and thickness of sediment layers (cells in the computational grid), the porosity of the sediment, the seepage velocity (Vseep), the bioturbation dispersion coefficient for solid substances (TurCoef) and the bio-irrigation dispersion coefficient for dissolved substances (DifCoef);
- a number of substances (sulphate, dissolved sulphide, particulate sulphide, apatite-phosphate, vivianite-phosphate, methane) and redox processes that are particularly relevant for sediment diagenesis (included in D-Water Quality's processes library);
- input parameters for these processes, such as kinetic coefficients;
- exchange fluxes between microphytobenthos biomass (GEMMPB) and benthic grazer biomass (CONSBL) modules and substances in the sediment;
- exchange fluxes for settling and resuspension between the lower water layer and the upper sediment layer;
- a numerical integration scheme for explicit integration in horizontal directions and implicit integration in the vertical direction (extended scheme 12).

Settling and resuspension fluxes and required input were already available in D-Water Quality. The initial composition of the sediment and the lower boundary concentrations for the sediment are specified in D-Water Quality's input in exactly the same way as for water com-

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partments. The same holds for simulation output.

D-Water Quality as based on the comprehensive configuration Delft3D-ECO for eutrophication modelling has now been tested extensively for cases with settling only, in which sediment layer thickness and sediment porosity are constant over time. A correct application was also made for organic micro-pollutants. Further testing needs to be done for resuspension, transient layer thickness, transient porosity and heavy metals. Transient porosity as based on consolidation formulations has not yet been implemented.

2.2 Mass transport in the sediment

At present only vertical mass transport is considered for bottom sediment. Vertical mass transport between the sediment layers, across the sediment-water interface and across the lower sediment boundary is calculated in D-Water Quality by a set of process routines integrated in D-Water Quality's processes library (AdvTra, DspTtr, TraSe2_X or TrSe2_X). Processes TraSe2_X (or TrSe2_X depending on the length of name X) are substance specific where X indicates the name of a simulated substance. Some of these names have been shorted to avoid the process name being longer than 10 characters (e.g. APAT and SAL in stead of APATP and Salinity). Like all processes in D-Water Quality these processes need to be activated in section 6 of D-Water Quality's input by means of Active_Y, where Y contains the full name of the process. An example is:

```
CONSTANTS       'ACTIVE_AdvTra'     DATA     1.00000e+000
CONSTANTS       'ACTIVE_DspTra'     DATA     1.00000e+000
CONSTANTS       'ACTIVE_TraSe2_AAP' DATA     1.00000e+000
```

Vertical mass transport processes in the sediment may include burial, digging, seepage, bioturbation, bio-irrigation, flow induced dispersion and molecular diffusion. Burial, digging and seepage (upwelling or downwelling) are forms of advection. Bioturbation of solid substances and bio-irrigation of dissolved substances are forms of dispersion. All dispersive processes are formulated as diffusion.

The burial of particulate substances results from net settling at the sediment-water interface, digging results from net resuspension at this interface. The advection of particulate substances by burial or digging follows from:

$$Fadv_p = \frac{vp \times fp \times C}{(1-\varphi)} \tag{2.1}$$

where:

C	bulk concentration of a substance [g m^{-3}]
$Fadv_p$	particulate advection flux [g m^{-2} d^{-1}]
fp	particulate fraction of a substance [-]
vp	volumetric burial or digging velocity [m d^{-1}]
φ	porosity [-]

Fraction fp is equal to 1.0, except for micro-pollutants. The model calculates *fp* for these substances as it depends on adsorption.

For fixed porosities and fixed layer thickness burial and digging imply transport fluxes across all the interfaces of the sediment layers. This includes the interface of the lower active sediment layer in the model and the deeper inactive sediment (boundary condition). The burial and digging velocities vp are calculated in the model from the settling and resuspension fluxes

in such a way that constant porosity in and constant thickness (volume) of each sediment layer is maintained. This uses the following definition of porosity:

$$\varphi = 1 - \sum_{i=1}^{n} \frac{fp_i \times C_i}{\rho_i} \tag{2.2}$$

where:

φ	porosity [-]
C_i	bulk concentration of a substance [g m^{-3}]
fp_i	particulate fraction of a substance [-]
ρ_i	density of a solid matter component [g m^{-2} d^{-1}]
i	index of a solid matter component [-]
n	number of solid matter components [-]

For transient layer thickness or for transient porosity the volumetric burial or digging velocity vp is the sum of an imposed velocity (input parameter, see Sections 2.3.3 and 2.3.6) and an additional velocity to maintain maximal layer thickness or minimal layer thickness. In the case of fixed porosity the additional velocity also serves to maintain porosity at its imposed value (see section 2.3.3). The additional velocity is calculated within the model.

Porosity φ is the input parameter *Porinp* (see section 2.3.4). *Porinp* can be used for fixed porosity (constant) as well as transient porosity (time series).

The settling fluxes for the water column are calculated according to the settling process described in D-Water Quality's Technical Reference Manual using input settling velocities. Resuspension can be simulated according to Partheniades-Krone formulations or De Boer formulations (input option parameter *SwErosion* is 0.0 or 1.0 respectively).

Seepage can be upwelling or downwelling (infiltration). It affects only the dissolved substances. Seepage implies transport fluxes across the sediment-water interface, the interfaces of the sediment layers, and the interface of the active sediment and the deeper inactive sediment. The seepage advection flux is:

$$Fadv_d = \frac{vd \times fd \times C}{\varphi} \tag{2.3}$$

where:

C	bulk concentration of a substance [g m^{-3}]
$Fadv_d$	dissolved advection flux [g m^{-2} d^{-1}]
fd	dissolved fraction of a substance [-]
vd	volumetric seepage velocity [m d^{-1}]
φ	porosity [-]

The fraction fd is equal to 1.0, except for micro-pollutants (calculated by the model as $1-fp$). The seepage velocity is the input parameter *Vseep* (see section 2.3.6), which has a negative value in the case of downwelling.

Bioturbation by benthic organisms causes the dispersion of particulate substances. The pertinent dispersion flux is approximated with:

$$Fdis_p = \max\left(1-\varphi_1, 1-\varphi_2\right) \times Dp \times \frac{\left(fp_1 \times C_1/\left(1-\varphi_1\right) - fp_2 \times C_2/\left(1-\varphi_2\right)\right)}{\left(L_1 + L_2\right)} \tag{2.4}$$

where:

C	bulk concentration of a substance [g m^{-3}]
Dp	particulate dispersion coefficient [m^2 d^{-1}]
$Fdis_p$	particulate dispersion flux [g m^{-2} d^{-1}]
fp	particulate fraction of a substance [-]
L	dispersion length [m]
φ	porosity [-]

indexes 1 and 2 refer to two adjacent sediment layers (grid cells)

The dispersion coefficient *Dp* is the input parameter *TurCoef* (see section 2.3.5). Each dispersion length *L* is the half thickness of the sediment layer concerned. The bioturbation flux is zero at the sediment-water interface.

Benthic organisms also cause bio-irrigation, the dispersion of dissolved substances. Water flow over the sediment causes micro-turbulence in the upper pore water, which is another source of dispersion. The overall dispersion coefficient includes the effects of bio-irrigation, flow and molecular diffusion. The dispersion of dissolved substances implies transport fluxes across the sediment-water interface. These fluxes include the so-called return fluxes of nutrients to the water column and the sediment oxygen consumption flux. The dispersion flux of a solute follows from:

$$Fdis_d = \min(\varphi_1, \varphi_2) \times Dd \times \frac{(fd_1 \times C_1/\varphi_1 - fd_2 \times C_2/\varphi_2)}{(L_1 + L_2)} \tag{2.5}$$

where:

C	bulk concentration of a substance [g m^{-3}]
Dd	diffusion or dispersion coefficient [m^2 d^{-1}]
$Fdis_d$	dissolved dispersion flux [g m^{-2} d^{-1}]
fd	dissolved fraction of a substance [-]
L	dispersion length [m]
φ	porosity [-]

indexes 1 and 2 refer to two adjacent sediment layers (grid cells)

The dispersion coefficient *Dd* is the input parameter *DifCoef* (see section 2.3.5). Each dispersion length *L* is the half thickness of the sediment layer concerned. For the sediment-water interface L_1 in the lower water layer is input parameter *Diflen*. The bio-irrigation flux is zero at the interface of the lower active sediment layer and the deeper sediment (lower boundary).

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2.3 Input specification

2.3.1 The sediment grid

Exchanging substances with the water body, the sediment bed is modelled with an additional computational grid. Each sediment layer is a flat relatively thin cell in this grid. Together the sediment layers form a sediment segment, which is in fact a sediment column. Each sediment segment is connected to a cell in the computational grid for the water body (water grid), namely the lower water layer of a water segment, which is in fact a water column. The

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set of sediment segments constitutes the sediment grid. This sediment grid must be defined using the MULTIGRID keyword just after the number of water segments in block 3 of the input file. The MULTIGRID part of the input consists of the input items described below as based on an input example. The MULTIGRID part of the input file must end with the keyword END_MULTIGRID.

The keyword ZMODEL indicates that the underlying hydrodynamic model uses a z-layer approach (fixed thickness). If omitted, a σ-layer or 2D model approach is assumed, for which layer thickness is relative to water depth.

The keyword NOLAY is to be followed by the number of water layers in the (aggregated) water grid.

Several sediment grid files can be defined in the input file, but the first one specified is the one that defines the computational grid for the sediment in the D-Water Quality simulation. The other grid files can be used for the specification of *input items*. The grid can be divided in zones. A zone comprises a number of sediment segments that have similar properties. Zones can be different as to the number of sediment layers and input items such as initial composition, temperature forcing, and process coefficients. Sediment segments as well as zones are identified by sequence numbers. The sediment segments must be sequentially numbered from 1 to M (the number of segments). The zones must be sequentially numbered from 1 to N (the number of zones).

The keyword BOTTOMGRID is used to identify the sediment grid and the various grid files. It is to be followed by the name of the sediment grid or a sediment zone. This combination is (optionally) followed by the keyword REFERENCEGRID and the name of the reference grid. This set of keywords can be repeated several times to further specify the sediment grid and the zones:

- ◇ The first keyword BOTTOMGRID is used to identify the sediment grid that defines the computational grid in the D-Water Quality simulation. It is followed by the name of the sediment grid. This combination is followed by the keyword REFERENCEGRID and the name of the reference grid. The reference grid is the water grid for which the sediment grid is specified. By default this is the (aggregated) grid of the water body in the model, and has the prescribed name ‘Base grid’.
- ◇ After this the specification of the sediment grid follows, which consists of a table with the numbers of the sediment segments for each water segment in the reference grid. The segment numbers must be assigned in the order of the water grid cells. That means that the first record is connected to water grid cell 1, and the last record is connected to water grid cell L (the number of water grid cells in a water layer). Water grid cells without a sediment bed must be assigned a zero in this table.
- ◇ The second keyword BOTTOMGRID defines the zoning of the sediment segments. It is followed by the name of the sediment grid to which zoning applies. The reference grid is usually the entire sediment grid. After this the specification of the zones follows, which consists of a table with the numbers of the zones for each sediment segment. The zone numbers must be allocated in the order of the sediment segments. That means that the first record is connected to segment 1, and the last record is connected to segment M.
- ◇ The third keyword BOTTOMGRID can be used to create a sediment zone that comprises all sediment segments, which can be conveniently called ‘sediment-default’. This zone can be used to allocate the same input item values to all segments. It is followed by a reference grid specification and value 1, which refers to the ‘Base grid’.

The keyword NOBOTTOMLAY is used to specify the number of layers in the sediment. The keyword must be followed by an additional keyword indicating for which segments the number

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of layers are specified:

- ◇ A possible keyword is ALL, which indicates that the number of layers given concerns all sediment segments. The keyword DEFAULT indicates that the default number of layers is applied to all sediment segments.
- ◇ If the sediment grid has zones, then the number of layers can be defined for each of the zones. This requires the keyword INPUTGRID placed immediately after NOBOTTOMLAY, followed by the name of the grid that has the zones and the number of the layers in each of the zones. The numbers of layers must be given in the order of the sequence numbers of the zones (number of layers for zone 1, number for zone 2, number for zone 3, etc.).

Zoning of the water body can be achieved by defining sub-grids with the keyword SUBGRID. The definition of a water sub-grid is analogous to the definition of a sediment zone sub-grid. A water sub-grid (zone) is only used to structure the input items such as the initial composition. The same value of an input item can be allocated to all cells in a sub-grid (zone). The keyword SUBGRID is followed by a name identifying the sub-grid (zone). This set is optionally followed by the keyword REFERENCEGRID with the name of the reference grid, on which the sub-grid is defined. The reference grid is by default the model grid which is called the 'Base grid', but it could also be a previously defined sub-grid. After the name the specification of the sub-grid follows which consists of a table with zone sequence numbers for each grid cell in the water grid. The zones must be allocated in the order of the grid cells in the water grid. That means that the first record is connected to grid cell 1. The last record is connected to grid cell L (the number of cells in a water layer).

A typical example of the specification of the sediment grid using included files is as follows:

```
#2          ; delimiter for the second block
;
; third block of model input (grid layout)
1212      ; number of grid cells in the water body (all water layers)
;
MULTIGRID
    ; z layer model with 4 layers
    ZMODEL
    NOLAY  4
    ; specification of the computational sediment grid
    BOTTOMGRID 'sediment-grid'
    REFERENCEGRID 'Base grid'
    INCLUDE '../model-input/grid/sediment-ag02.dwq'
    ; allocation of the segments to zones
    BOTTOMGRID 'sediment-zone'
    REFERENCEGRID 'sediment-grid'
    INCLUDE '../model-input/grid/sediment-zone-ag02.dwq'
    ; specification of a default zone
    BOTTOMGRID 'sediment-default'
    REFERENCEGRID 'sediment-zone'
    INCLUDE '../model-input/grid/sediment-default.dwq'
    ; all sediments segments have 7 layers, this example has 1 zone
    NOBOTTOMLAY INPUTGRID sediment-default 7
    ; allocation of the water grid cells to one zone for input purposes
    SUBGRID 'water-zone'
    INCLUDE '../model-input/grid/water-zone-ag02.dwq'
END_MULTIGRID
```

In the resulting overall computational grid, as created from the specifications in the input file, the sediment segments are placed after the water grid cells, and sediment boundaries are added for each sediment segment. If the number of sediment layers is the same for all

sediment segments, the numbering of the grid cells for K water layers and P sediment layers proceeds as follows:

- ◇ The grid cells in the top water layer run from 1 to L. The grid cells in the second water layer are numbered from 1+L to 2*L (etc.). The grid cells in the lower water layer are numbered from 1+(K-1)*L to K*L. The grid cells in a water segment (column) are numbered n, n+L, n+2*L, ..., n+(K-1)*L.
- ◇ The grid cells in the top sediment layer run from K*L+1 to K*L+P*M. The grid cells in the second sediment layer are numbered from K*L+1+M to K*L+2*M (etc.)., The grid cells in the lower sediment layer are numbered from K*L+1+(P-1)*M to K*L+P*M. The grid cells in a sediment segment (column) are numbered n+K*L, n+K*L+M, n+K*L+2*M, ..., n+K*L+(P-1)*M.

Notice that M is equal to L when each water segment (column) has a sediment segment (column).

2.3.2 Sediment boundaries

"Deep" sediment boundaries are added automatically. If the water grid has B boundaries, DELWAQ will number the sediment boundaries conform the sediment segment numbering from B+1 to B+M. The first boundary belongs to sediment grid cell K*L+1+(P-1)*M of grid segment 1. The last sediment boundary belongs to sediment grid cell K*L+P*M of grid segment M.

The definition of the names sediment boundaries follows the rules for water boundaries as described in Deltares (2026a). In the input file it must appear in block 5 immediately after the names of all water boundaries. Names are user determined. An example for M is 10 looks as follows:

```
#4          ; delimiter for the fourth block
;
; specification of names of water boundaries
;

;
; specification of names of sediment boundaries
;
'sedbnd0001'    'sedbnd0001'    'sedimentbound'
'sedbnd0002'    'sedbnd0002'    'sedimentbound'
'sedbnd0003'    'sedbnd0003'    'sedimentbound'
'sedbnd0004'    'sedbnd0004'    'sedimentbound'
'sedbnd0005'    'sedbnd0005'    'sedimentbound'
'sedbnd0006'    'sedbnd0006'    'sedimentbound'
'sedbnd0007'    'sedbnd0007'    'sedimentbound'
'sedbnd0008'    'sedbnd0008'    'sedimentbound'
'sedbnd0009'    'sedbnd0009'    'sedimentbound'
'sedbnd0010'    'sedbnd0010'    'sedimentbound'
```

Concentrations must be allocated to the simulated substances for the sediment boundaries. This allocation proceeds in the same way as for water boundaries, starting with keyword ITEM followed by the name of an individual boundary(e.g. 'sedbnd0001'), or the name of a boundary zone (e.g.'sedimentbound'). The concentrations of the particulate substances should be approximately equal to the concentrations of the same substances in the lower sediment layer.

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2.3.3 Sediment layer thickness

The thicknesses of the sediment layers are to be defined in block 7 of D-Water Quality's input. Fixed layer thickness applies when input option parameter *SWSediment* is equal to zero (default value). If *SWSediment* is equal to 1.0, layer thickness will be transient (variable).

For layer thickness three parameters can be defined. *FixTh* is used to quantify fixed layer thicknesses. MaxTh and MinTh specify the maximal and minimal layer thickness in the case of transient layer thickness. Layer thickness is to be specified as a parameter for each sediment layer in a sediment zone, or for each sediment layer in a sediment segment when zoning is not applied (see also section 2.3.1). The unit is meter. The specification for a zone requires the keyword `INPUTGRID` followed by the name of a zone (sub-grid). The sequence of the various keywords and the data for thickness follows from the following example:

```
PARAMETERS  'fixth'   INPUTGRID  'sediment-zone'
DATA
0.001       ; layer 1
0.002       ; layer 2
0.003       ; layer 3
0.006       ; layer 4
0.018       ; layer 5
0.07        ; layer 6
0.1         ; layer 7
```

In the case of steep concentration gradients the top layer should be 0.001 m thick. This is a feasible minimal value in order not to get unacceptably large computational burden (simulation run time) due to a very small timestep for integration. With such a top layer the timestep will mostly be between 2 and 5 minutes. The thickness of the other layers should increase with depth, in order to not have too many layers, which will also cause unacceptable computational burden. The overall thickness of the active sediment layer is 0.1–0.2 meter in fresh water systems, and 0.3–0.4 m in saline and brackish water systems.

2.3.4 Porosity and initial sediment composition

Like any input parameter in block 7 of the input the porosity *Porinp* (m^3water/m^3bulk sediment) can be provided as a constant, a parameter, a time function, or a segment function. It is recommended to use a constant or a parameter, for D-Water Quality has not yet been fully tested for the porosity varying over time. In the case of a parameter, the porosity is quanitified for each layer (grid cell) in each sediment zone or each sediment segment. See section 2.3.3 for a typical example of parameter specification.

The porosity is made equal to the input value if *Porinp* is larger than 10^{-4}. A smaller input value can be used to inform the model that porosity will be transient (variable over time) as simulated by the model. The initial porosity is then derived from the initial composition (imposed concentrations of particulate substances). However, the option for transient computed porosity would require consolidation formulations, which have not been implemented yet.

Realistic values for the porosity in a sediment bed are in between 0.35 (pure sand) and 0.9 (peat or peaty silt). A silt sediment has a porosity of approximately 0.7.

2.3.5 Dispersive transport

The dispersion coefficients TurCoef for particulate matter and Difcoef for solutes need to be specified in block 7 as a constant, a parameter, a time function or a segment function. It is recommended to specify these coefficients as segment functions (both space and time

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dependent) for each sediment zone or for each sediment segment. The bioturbation and bio-irrigation coefficients vary seasonally, dependent on the activity of benthic organisms. A typical example for input for a segment function is:

```
SEG_FUNCTIONS
DIFCOEF
INPUTGRID    `sediment-zone'
DATA
;
;                        Layer 1    Layer 2     Layer 3    Layer 4    Layer 5    Layer 6    Lay
;
2004/01/01-00:00:00    3.00E-04   3.00E-04    3.00E-04   3.00E-04   3.00E-04   1.00E-04   5.00
2006/12/31-00:00:00    3.00E-04   3.00E-04    3.00E-04   3.00E-04   3.00E-04   1.00E-04   5.00
```

TurCoef affects mass transport across all sediment interfaces, except for the sediment-water interface. The first given value concerns the interface between the top sediment layer and the second layer. A representative summer value for *TurCoef* near the sediment-water interface for a shallow freshwater system is 2.0×10^{-6} m^2/day. The winter value can be 10 % of the summer value. Bioturbation can be significantly faster in marine sediments. *TurCoef* decreases exponentially with depth, and is practically equal to zero at depths below 0.1 m in freshwater systems, and below 0.4 m in marine water systems.

DifCoef affects mass transport across all sediment interfaces, except for the lower sediment boundary. Any value given for this interface will be ignored. The first given value concerns the sediment-water interface. A representative summer value for *DifCoef* near the sediment-water interface for a shallow freshwater system is 5.0×10^{-4} m^2/day. This value is the sum of bio-irrigation, flow induced dispersion and molecular diffusion. The winter value can be 20% of the summer value. Bio-irrigation can be significantly faster in marine sediments. *DifCoef* decreases exponentially with depth, and is practically equal to the molecular diffusion coefficient corrected for tortuosity (φ^2) at depths below 0.1 m in freshwater systems, and below 0.4 m in marine water systems. A representative value for the corrected molecular diffusion coefficient is 0.25×10^{-4} m^2/day.

The dispersion length at the water side of the sediment-water interface *Diflen* can usually be provided as a constant value between 0.0005 and 0.001 m.

2.3.6 Advective transport

The seepage velocity *Vseep* (m/day) is the only advection parameter needed in input block 7 when layer thickness and porosity are both fixed. Burial and digging are calculated within the model. A positive value of *Vseep* will cause an upward transport, a negative value a downward transport. Vseep can be specified as as a constant, a parameter (example in section 2.3.4), a time function or a segment function (example in section 2.3.5). In the cases of a parameter and a segment function *Vseep* can be specified for each sediment zone or for each sediment segment. An typical example of a time function is:

```
FUNCTIONS
VSEEP
BLOCK
DATA
;
2009/01/01-00:00:00     0.01
2010/12/31-00:00:00     0.01
```

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In the case of transient layer thickness the volumetric burial and digging velocity needs to be provided as input parameter *VburDM* (m/day).

2.3.7 Process coefficients

All coefficients of water and sediment quality processes are specified in D-Water Quality's Technical Reference Manual and in updated process descriptions. All coefficients are specified in block 7 of the input as a constant, a parameter, a time function or a segment function. Values can be different for water grid cells and sediment grid cells. Some parameters can even vary among sediment grid cells. This holds in particular for:

- ◇ *RcNit20* , the nitrification rate at 20 °C
- ◇ *fr_FeIM1* , the fraction of reactive iron in sediment fraction IM1
- ◇ *fr_FeIM2* , the fraction of reactive iron in sediment fraction IM2
- ◇ *fr_FeIM3* , the fraction of reactive iron in sediment fraction IM3
- ◇ *fr_Feox* , the fraction of oxidised iron in total iron under reducing conditions
- ◇ *KadsP_20* , the adsorption equilibrium constant for phosphate
- ◇ *CoxDenInh* , the inhibition concentration of oxygen for denitrification
- ◇ *pH_min*, the minimal pH
- ◇ *pH_max*, the maximal pH

In the cases of a parameter and a segment function a coefficient can be specified for each sediment zone or for each sediment segment. A typical example of a parameter that is different for the water column and the sediment is:

```
;                                        water grid cells     sediment grid cells
PARAMETERS  RcNit20    ALL    DATA           820*0.1                  126*40.0
```

The number of sediment grid cells is the sum of the numbers of layers in each of the sediment segments.

2.4 Output specification

All output items are essentially the same for water grid cells and sediment grid cells, implying that (additional) output parameters need to be specified only once. *Poros* is the name of the output parameter for porosity. Like for water grid cells, the output concentrations for sediment grid cells are bulk concentrations in g/m^3. The concentrations of solutes in pore water can be derived from the bulk concentrations by dividing bulk concentrations by porosity.

All output of sediment grid cells are added to the standard map output. Sediment segments can be added as monitoring point or area for monitoring, history and balance output. A monitoring point or area can be excluded from the balance output by adding the keyword `NO_BALANCE` directly after the name of the monitoring point or area.

Process fluxes in the balance output are dealt with in the same way for water and sediment compartments. All parts of the sediment water interaction are lumped and reported in the balance as transport, because the net flux is calculated by the D-Water Quality transport solver. If the user wants output for the individual sediment-water exchange fluxes, he is advised to include both the water and the sediment compartment as a monitoring point or area, in combination with the balance option “not lump internal transport”.

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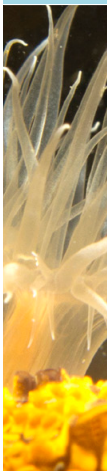
References

Deltares, 2026a. *D-Water Quality Description of Input file*. Deltares, 2.00 ed.

Deltares, 2026b. *D-Water Quality Technical Reference Manual*. Deltares, 5.01 ed.

Deltares, 2026c. *D-Water Quality User Manual*. Deltares, 5.06 ed.



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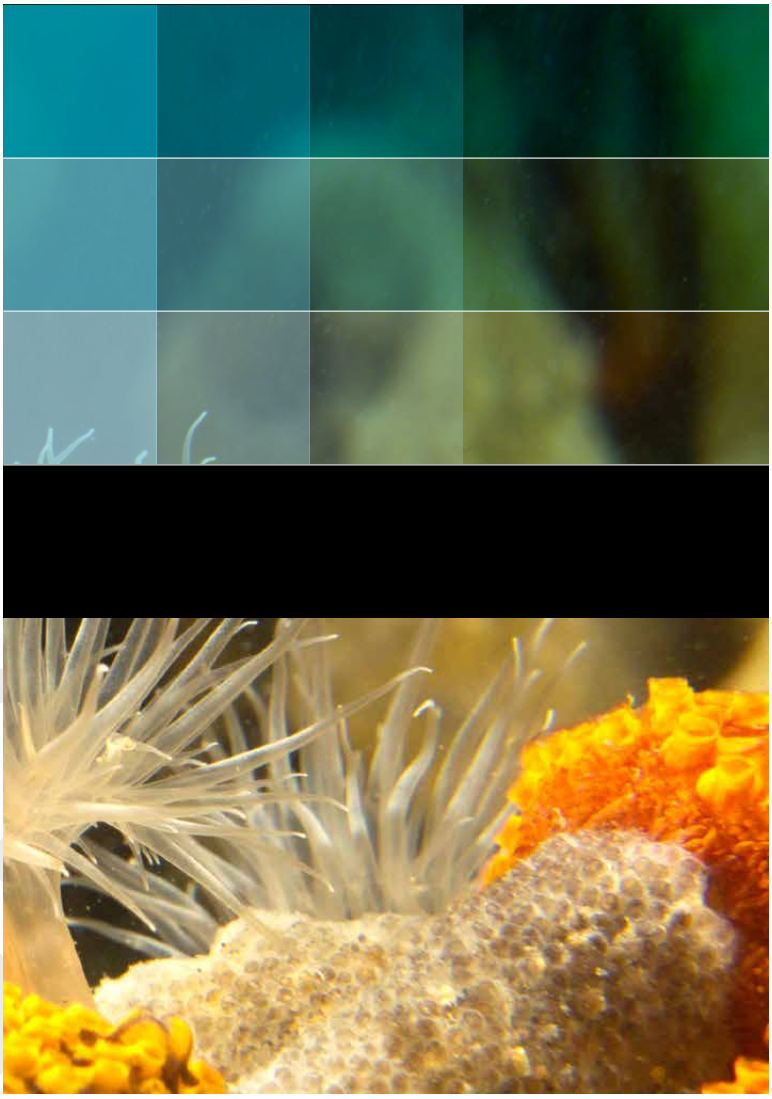

Photo by: Mathilde Matthijsse, www.zeelandonderwater.nl

s systems

+31 (0)88 335 81 88
sales@deltaressystems.nl
www.deltaressystems.nl

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