

Simulation software for safe, sustainable and future deltas

DELFT3D FM SUITE 2D3D

Deltares systems

D-Water Quality

D-Water Quality

Versatile water quality modelling

User Manual

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Contents

List of Tables	ix
List of Figures	xi
1 A guide to this manual	1
1.1 Introduction	1
1.2 Overview	1
1.3 Manual version and revisions	2
1.4 Typographical conventions	2
1.5 Glossary	3
1.6 Changes with respect to previous versions	4
2 D-Water Quality: Overview	5
2.1 Introduction	5
2.1.1 About water quality modelling and D-Water Quality	5
2.1.2 What is a D-Water Quality model?	5
2.1.3 The main features of the GUI	7
2.1.4 The D-Water Quality computational core	8
2.2 Schematisations & hydrodynamics	8
2.3 The Processes Library	9
2.4 More information	10
3 D-Water Quality: Getting started	11
3.1 Starting a model	11
3.2 Setting up a fraction simulation	13
3.3 Working with coordinate systems and a background map	16
3.4 Setting up a water quality simulation	17
4 D-Water Quality: All about the modelling process	25
4.1 Starting a model and Importing the geometry and flow data from an existing hydrodynamics model	25
4.1.1 Grid definition	25
4.1.2 Segment properties	26
4.1.3 Exchanges and exchanges properties	27
4.1.4 Vertical dispersion	27
4.1.5 Time frames	27
4.1.6 Available links to hydrodynamics models	28
4.1.7 Finding a particular segment	28
4.2 The D-Water Quality input file	28
4.3 General water quality model properties	29
4.4 Simulation and Output timers	30
4.5 Numerical options	31
4.6 Add a definition of substances and processes	33
4.6.1 The PLCT (Processes Library Configuration Tool)	33
4.7 Set initial conditions	34
4.7.1 Spatial fields	34
4.7.2 Restarting	34
4.8 Set process coefficients (including meteo data)	34
4.8.1 Time functions	35
4.8.2 Spatial fields	36
4.8.3 Link to hydro data	37
4.8.4 Coefficients for the BLOOM algae sub model	37
4.9 Dispersion coefficients	37

4.9.1	Horizontal dispersion	37
4.9.2	Vertical dispersion	38
4.10	Pollution loads	39
4.10.1	Properties	39
4.10.2	Importing pollution loads	39
4.10.3	Loads corresponding to sources in the hydrodynamics model	39
4.11	Observation point	40
4.11.1	Properties	40
4.11.2	Importing observation points	40
4.12	Observation areas	41
4.12.1	Define observation areas manually	41
4.12.2	Define observation areas from an imported shape file	41
4.13	Boundary conditions and loads data	41
4.13.1	Boundaries and loads	42
4.13.2	Functionality of the input processor	42
4.13.3	Working with data sets	43
4.13.4	Supported data set formats	44
4.13.5	Substance aliases ("USEFOR rules")	45
4.13.6	Location aliases	46
4.13.7	Load types; setting defaults	47
4.14	Mass balances	47
4.15	Run simulation	48
4.15.1	Model validation	49
4.15.2	Troubleshooting	49
4.16	Postprocessing	50
4.16.1	Using Delft3D Flexible Mesh Suite or D-HYDRO Suite.	50
4.17	Project, model and file management	50
5	Conceptual description	51
5.1	Introduction	51
5.2	Mass balances	51
5.3	Spatial schematisation	52
5.4	Advection-diffusion equation	54
5.4.1	Advective transport	54
5.4.2	Dispersive transport	55
5.4.3	Transport from sources	55
5.4.4	Mass transport by advection and dispersion	56
5.5	Boundary conditions	58
5.5.1	Closed boundaries	58
5.5.2	Open boundaries	58
5.5.3	Time lags and return time	58
6	Principles of water quality modelling	61
6.1	Introduction	61
6.2	Salinity, chloride, tracers and continuity	61
6.3	Water temperature and temperature dependency of rates	62
6.4	Coliform bacteria	63
6.4.1	Concepts	63
6.4.2	Modelling framework	64
6.4.3	Process equation	64
6.5	Dissolved oxygen and BOD	65
6.5.1	Concepts	65
6.5.2	Modelling framework	67
6.5.3	Process equations	70

6.6	Suspended sediment, sedimentation and erosion	72
6.6.1	Concepts	72
6.6.2	Modelling framework	74
6.6.3	Processes	77
6.7	Nutrients, detrital organic matter and electron-acceptors	84
6.7.1	Concepts	84
6.7.2	Modelling framework	85
6.7.3	Process equations	99
6.8	Primary producers: phytoplankton	106
6.8.1	Concepts	106
6.8.2	Modelling framework	108
6.8.3	Process equations	113
6.9	Primary consumption	117
6.9.1	Concepts	117
6.9.2	Modelling framework	118
6.9.3	Process equations	120
6.10	Heavy metals and organic micro-pollutants	122
6.10.1	Concepts	122
6.10.2	Modelling framework	122
6.10.3	Process equations	126
6.11	Sediment modelling	129
6.11.1	Concepts	130
6.11.2	Modelling framework	133
6.11.3	Process equations	134
7	Numerical aspects	137
7.1	Dispersion and turbulent diffusion	137
7.2	Introduction to algorithmic implementation	141
7.3	Conceptual description	142
7.3.1	Partial differential equations	142
7.3.2	Differential equations for computational cells	142
7.4	Numerical discretisation	144
7.4.1	Introduction	144
7.4.2	Time discretisation and stability criteria	145
7.4.3	Discretisation of transport and numerical diffusion	146
7.5	Numerical schemes in D-Water Quality	148
7.5.1	Upwind scheme (Scheme 1)	150
7.5.2	Second order Runge-Kutta (Scheme 2), Lax Wendroff method (Scheme 3) and Alternating Direction Implicit (2D) method (Scheme 4)	151
7.5.3	Flux Correct Transport (FCT) Method (Scheme 5)	151
7.5.4	Steady-state solutions (Schemes 6 to 9, 17 and 18)	151
7.5.5	Implicit Upwind scheme with a direct solver (Scheme 10)	152
7.5.6	Horizontal Upwind scheme, Vertical: implicit in time and central discretisation (Scheme 11)	152
7.5.7	Horizontal: FCT scheme, Vertical: implicit in time and central discretisation (Scheme 12)	152
7.5.8	Horizontal: Upwind scheme, Vertical: implicit in time and upwind discretisation (Scheme 13)	153
7.5.9	Horizontal: FCT scheme, Vertical: implicit in time and upwind discretisation (Scheme 14)	153
7.5.10	Implicit Upwind scheme with an iterative solver (Scheme 15)	153
7.5.11	Implicit Upwind scheme in horizontal, centrally discretised vertically, with an iterative solver (Scheme 16)	154

7.5.12	ADI scheme for 3D models (horizontal: higher order scheme, vertical: central and upwind discretisation (Schemes 19 and 20)	155
7.5.13	Local-theta flux-corrected transport scheme (Scheme 21 and 22)	155
7.5.14	QUICKEST scheme (Scheme 23)	155
7.5.15	Flux-corrected transport with adaptive time-stepping (scheme 24)	155
7.6	Artificial vertical mixing due to σ co-ordinates	156
References		161
A File descriptions		165
A.1	Overview of files	165
A.2	Description of file formats	168
A.2.1	Binary files	168
A.2.1.1	History files (.his)	168
A.2.1.2	Map files (.map)	169
A.2.1.3	Segment function files	170
A.2.1.4	NetCDF files	170
A.2.1.5	NEFIS files	170
A.2.2	CSV files for input	170
B The hyd-file		173
B.1	Contents of the hyd-file	173
B.2	UGRID files that are directly read by D-Water Quality	176
B.3	ASCII files that are directly read by D-Water Quality	177
B.4	Binary files that are directly read by D-Water Quality	177
C Standard substance files		179
C.1	Introduction	179
C.2	Salinity and tracers (fractions)	179
C.2.1	General	179
C.2.2	Introduction	179
C.2.3	Description of processes	180
C.2.4	Notes	180
C.2.5	Output items	180
C.3	Basic coliform model	180
C.3.1	General	181
C.3.2	Introduction	181
C.3.3	Description of processes	182
C.3.4	Notes	183
C.3.5	Output items	184
C.4	Basic dissolved oxygen model	184
C.4.1	Introduction	184
C.4.2	Description of processes	186
C.4.3	Notes	188
C.4.4	Output items	188
C.5	Basic suspended sediment model	188
C.5.1	General	188
C.5.2	Introduction	188
C.5.3	Description of processes	189
C.5.4	Inorganic Matter (suspended and settled)	189
C.5.5	Notes	191
C.5.6	Output items	191
C.6	References	191
D Statistical output functions		193

D.1	Descriptive statistical parameters (stadsc)	193
D.2	Geometric mean (stageo)	193
D.3	Depth-average mean (stadpt)	194
D.4	Periodical mean (staday)	194
D.5	Quantiles (staqtl)	194
D.6	Percentage exceedance (staprc)	195
E	User-defined wasteloads	197
E.1	Introduction	197
E.2	IT-background	197
E.3	The dynamic link library	197
E.4	delwaq_user_wasteload subroutine	198
E.5	“wasteload” derived type	198
E.6	Utility function find_wasteload	199
E.7	Utility function find_substance	199
E.8	Recapitulation	200
E.9	Example source code delwaq_user_inlet_outlet	200

DRAFT

List of Tables

6.1	Typical values for oxygen demanding waste waters (values in g O ₂ /m ³ , data from Thomann and Mueller (1987))	67
6.11	Major processes for ammonium, nitrate, phosphate and silica as occurring in sediment layers	131
7.1	Common ranges of horizontal dispersion terms in aggregated models with a finite grid	141
A.1	Files in D-Water Quality	165
B.1	Dimensions mentioned in table B.2	177
B.2	Documentation of the binary input files that can be read directly by D-Water Quality	178

DRAFT

List of Figures

3.1	<i>Import</i> button in ribbon	12
3.2	Select type of data window	12
3.3	File selection window	12
3.4	View of horizontal aggregated imported model	13
3.5	Substances representing fractions	14
3.6	Boundary concentration for "SEA BOUNDARY"	14
3.7	Results of "SEA BOUNDARY" after one tidal cycle	15
3.8	Results of initial value after one tidal cycle	16
3.9	Property window	16
3.10	Add new WMS layer	17
3.11	Select the appropriate WEB link	17
3.12	Result after selecting the WEB link	17
3.13	Import a substances or processes configuration file window	18
3.14	Set initial values	19
3.15	Set processes coefficients	19
3.16	Set the dispersion coefficient	19
3.17	Set an additional homogeneous vertical dispersion coefficient	20
3.18	Showing the names of the added observation points	21
3.19	Import boundary conditions	21
3.20	Import waste load data	22
4.1	D-Water Quality grid definition	25
4.2	General parameters, σ -layer model	26
4.3	View on D-Water Quality input file	28
4.4	General water quality model properties	29
4.5	Simulation and Output timers	30
4.6	Numerical options	31
4.7	Substances file import wizard	33
4.8	Spatial fields	34
4.9	Indication in project explorer of initial conditions for NH_4	34
4.10	Restart parameters	34
4.11	Time functions	35
4.12	Indication in project explorer of process coefficients fSOD and VWIND	35
4.13	Time series editor	36
4.14	Spatial fields	36
4.15	Indication in project explorer of time dependent process coefficient VWIND	37
4.16	Coefficients for the BLOOM algae sub model	37
4.17	Horizontal dispersion	37
4.18	Indication in project explorer of horizontal dispersion <i>Dispersion</i>	38
4.19	Dispersion options (horizontal)	38
4.20	Dispersion options (vertical)	38
4.21	Observation points	40
4.22	Observation areas operation parameters	41
4.23	Edit polygon option in ribbon	41
4.24	Showing import result of a dataset	43
4.25	Location aliases for boundaries	46
4.26	Location aliases for load data	46
4.27	Setting default values for Load types	47
4.28	Balance options	47
4.29	Model validation result	49

5.1	Division of a lake into small boxes with a finite volume; a structured three dimensional grid is used	52
5.2	Schematisation of an estuary with 11 computational cells and 5 boundary cells	53
5.3	Thatcher-Harleman boundary time lag	59
6.1	General overview of substances included in D-Water Quality	61
6.2	Overview of substances. Coliform bacteria	63
6.3	Overview of substances. Dissolved oxygen and BOD	65
6.4	The distribution of gross primary production over a day	71
6.5	Overview of substances. Suspended sediment, sedimentation and erosion . .	73
6.6	Overview of substances. Nutrients, detrital organic matter and electron-acceptors	84
6.7	Overview of substances. Primary producers: phytoplankton	106
6.8	Overview of substances. Primary consumption	118
6.9	Overview of substances. Heavy metals and organic micro-pollutants	122
6.10	Overview of substances. Substances that are considered in the S1-S2 approach for sediment are encircled.	130
7.1	Estuary represented as a 1-dimensional model	138
7.2	Effect of turbulent fluctuations Δv_x on the net transport	139
7.3	“Dispersion” by inhomogeneity of flow in a cross-sectionally averaged one-dimensional model	140
7.4	Finite Volume for diffusive fluxes and pressure gradients	157
7.5	Left and right approximation of a strict horizontal gradient	158

1 A guide to this manual

1.1 Introduction

This User Manual concerns the water quality module D-Water Quality.

This module is part of several Modelling suites, released by Deltares as Deltares Systems or Dutch Delta Systems. These modelling suites are built with use of the Delta Shell framework. The framework enables to develop a range of modeling suites, each distinguished by the components and — most significantly — the (numerical) modules, which are plugged in. The modules which are compliant with the Delta Shell framework are released as *D-Name of the module*, for example: D-Flow Flexible Mesh, D-Waves, D-Water Quality, D-Real Time Control and D-Rainfall Runoff.

Therefore, this User Manual is shipped with several modelling suites. On the *Start Page* links are provided to all relevant User Manuals (and Technical Reference Manuals) for that modelling suite. Other user manuals can be referenced. In that case, you need to open the specific user manual from the *Start Page* in the central window. Some texts are shared in different user manuals, in order to improve the readability.

1.2 Overview

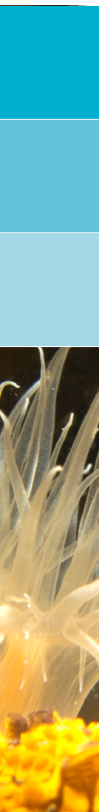
Working with any simulation package requires knowledge. We distinguish three types that are required for modelling of water quality:

- 1 Theoretical knowledge on water quality processes in natural systems.
- 2 Knowledge on how to operate the Delft3D or SOBEK software tools: the Graphical User Interface, visualisation of results, etc.
- 3 Numerical and mathematical knowledge on modelling and the simulation package.

The level of knowledge you need, depends on what you intend to do with the water quality model. Usually there is no need to be a theoretical water quality expert, but a decent level of knowledge is required to be able to understand the rather complex interaction of processes and to assess the correctness and suitability of the result. Remember that due to numerical artefacts or inadequate input models can do predictions that are not realistic. It is up to the modeller to recognise this and to reject the simulation results. For example, a dissolved oxygen concentration of 100 mg/l should make you extremely suspicious as the normal range is 0 to 20 mg/l. If you have a suitable water quality background, D-Water Quality could be a feast of recognition for you!

Obviously, working with D-Water Quality requires you to have knowledge on how to work with the software. Basically this involves knowing which buttons to press, where to enter which input item, and how to format data to be used in the water quality modelling.

Finally, theoretical water quality knowledge has been synthesised in mathematical formulations. Additionally the flow of water and the way it transports substances through a water system makes *advection and dispersion* (i.e. transport) an essential and vital part of modelling water quality in natural systems (think of a river discharging nutrients and suspended matter into the sea). Water quality modelling in D-Water Quality involves numerically solving the so-called advection-dispersion-reaction equation. Knowledge on the principles of this equation and its implementation in D-Water Quality is necessary. Numerical skills are not required as D-Water Quality will solve the equation for you, but you should be able to recognise numerical artefacts.



If you are not familiar with the theoretical water quality discipline, we advise you to start with the concepts on water quality modelling ([Chapter 5](#)) and the principles of water quality ([Chapter 6](#)) and even to study a handbook such as:

- ◇ [Chapra \(1996\)](#)
- ◇ [Thomann and Mueller \(1987\)](#)
- ◇ [Chapman \(1996\)](#)
- ◇ [Laws \(1993\)](#)

If you are a more experienced water quality modeller, the concepts in [Chapter 5](#) are a good starting point as well and you will probably understand quickly the background of D-Water Quality.

After that, you should start with the tutorial in [Chapter 3](#) as it will guide you through the screens and the basic functionalities of the D-Water Quality framework, without overwhelming you with a lot of details and the many possibilities and alternatives D-Water Quality contains.

The remaining chapters and appendices provide you with detailed information and can be checked whenever you need more information on a specific subject. Once you are familiar with the concepts of water quality modelling with D-Water Quality, these chapters and appendices will be your guide to further optimise your use of D-Water Quality.


1.3 Manual version and revisions

This manual applies to the D-Hydro Suite, version 2016 and later, the Delft3D Flexible Mesh Suite, version 2016 and later and the SOBEK 3.4 Suite and later.

1.4 Typographical conventions

Throughout this manual, the following conventions help you to distinguish between different elements of text.

Example	Description
Module Project	Title of a window or a sub-window are in given in bold . Sub-windows are displayed in the Module window and cannot be moved. Windows can be moved independently from the Module window, such as the Visualisation Area window.
<i>Save</i>	Item from a menu, title of a push button or the name of a user interface input field. Upon selecting this item (click or in some cases double click with the left mouse button on it) a related action will be executed; in most cases it will result in displaying some other (sub-)window. In case of an input field you are supposed to enter input data of the required format and in the required domain.
<\tutorial\wave\swan-curvi> <siu.mdw>	Directory names, filenames, and path names are expressed between angle brackets, <>. For Linux environments a forward slash (/) is used instead of the backward slash (\) for Windows environments.

Example	Description
"27 08 1999"	Data to be typed by you into the input fields are displayed between double quotes. Selections of menu items, option boxes etc. are described as such: for instance 'select Save and go to the next window'.
delft3d-menu	Commands to be typed by you are given in the font Courier New, 10 points.
	In this User manual, user actions are indicated with this arrow.
[ms ⁻¹] [-]	Units are given between square brackets when used next to the formulae. Leaving them out might result in misinterpretation. Most units will be in SI notation. [m AD] stands for 'meter Above Datum', which denotes a level relative to the vertical reference system in the model.

1.5 Glossary

We include here a glossary for several reasons. First, some words will occur frequently in the text and a quick reference guide could be useful. Second, in the D-Water Quality modelling terminology some words may have a slightly different meaning than you are used to. Hence it is important to realise their definition. Third, throughout the manual specific terms related to the model will be introduced. These terms are compiled here for easy reference.

Substance	A D-Water Quality state variable. D-Water Quality models the transport of active substances by solving the advection-diffusion equation numerically. The concentration of in-active substances is not affected by advective or dispersive transport. The D-Water Quality process-library contains water quality and transport processes. The concentration of active and inactive substances can be affected by water quality processes.
Active (substance)	Active substances are substances that can be transported by the flow of water, thus dissolved and particulate material in the water column.
Inactive (substance)	Inactive substances are substances that can not be transported by the flow of water. Substances that are part of the sediment are inactive substances.
Process	Processes can be divided into water quality processes and transport processes. A water quality process is associated with the transformation of substances (e.g. nitrification or mineralisation) and it generates one or more <i>fluxes</i> . A transport process is associated with the redistribution of substances and it generates one or more <i>velocities</i> or <i>dispersions</i> (e.g. sedimentation or vertical dispersive transport in a stratified water system). A process may also generate <i>process output</i> . Some processes calculate process output solely, e.g. the calculation of the extinction of light.
Process output	Fluxes, velocities and dispersions influence the concentration of specific <i>substances</i> . In case of a water quality process the calculated flux is linked to the related substance through a stoichiometric rela-

	tion.
Flux	A change of mass per unit of time and volume connected to a specific water quality <i>process</i> (for example the nitrification flux is the amount of ammonium converted to nitrate per unit of time and volume).
Segment related and exchange related information	<i>Process input</i> and <i>process output</i> is divided into segment related and exchange related information. Segment related information is known for each <i>segment</i> of the schematisation (e.g. parameters). Exchange related information is known for each <i>exchange area</i> of the schematisation (e.g. additional velocities).
Segment	Computational element of the water quality schematisation of the study area.
Exchange	The D-Water Quality model considers computational elements (or <i>segments</i>) as volumes that are linked to each other. The links or exchanges are defined by the segment number on both sides of the contact area.
Exchange area	The contact area of two linked computational elements (or <i>segments</i>).
Segment function	File (usually binary) that contains information for an input parameter that varies in time and space.
Constant	Input parameter that does not vary in time nor in space.
BLOOM	A Deltares software program to model multi-species algae growth and mortality. D-Water Quality contains an interface to BLOOM in the form of the process D40BLO.
CONSBL	A process module of the Processes Library of D-Water Quality to model grazing of phytoplankton and detritus on the basis of grazer biomass forcing.
Parameter	An input item that varies in space.
Function	An input item that varies over time.

1.6 Changes with respect to previous versions

This is the first edition which is published.

2 D-Water Quality: Overview

2.1 Introduction

2.1.1 About water quality modelling and D-Water Quality

Water quality modelling is a proven and accepted tool to support water quality management and integrated water management. It answers questions like: Which are the causes of existing water quality problems in a given water system? What are the effects of the current water management policy? What can be expected if we implement alternative policies? Which policy is the most effective? Etc.

D-Water Quality allows you to build water quality models for fresh, brackish and saline water systems, on the basis of a pre-existing hydrodynamic model (built with Delft3D-FLOW, D-Flow Flexible Mesh, SOBEK-FLOW, etc.). D-Water Quality is so flexible that it can be used in a 1D, 2D, 3D context, using structured and unstructured grids, but also in a multi-compartment catchment modelling context.

2.1.2 What is a D-Water Quality model?

A mathematical water quality model delivers an approximate quantitative description of one or more water quality "state variables" in a given water system. A model provides an imperfect image of reality, and is as accurate as needed or as possible. Details depend on modelling objectives and the available data. For meaningful water quality modelling, insight in the limitations and the accuracy of the model used is required.

In D-Water Quality models the "state variables" are "substances" that represent a pollutant, a naturally present substance or an aquatic organism. Substances may enter the modelled area through model boundaries, lateral in flows or "dry" waste loads. Unless attached to or located in the sediment bed, they move with currents and turbulence through the modelled water body (model domain). Water flow and dispersion coefficients are usually derived from a hydrodynamic model (for instance Delft3D-FLOW, D-Flow Flexible Mesh or SOBEK-FLOW). At the same time the substances show their own specific behavior in the aquatic environment. This can be a simple decay, but also one or more transformations in interaction with other substances. Most transformations are due to microbial organisms, phytoplankton and other aquatic organisms. Some processes are chemical reactions. Other processes are physical, such as the transfer between water and atmosphere. The rates of all water quality processes are formulated according to simplified or advanced kinetic rules, each requiring input parameters, often indicated as process coefficients. The rates are dependent on temperature, and sometimes other meteorological parameters such as solar radiation and wind speed. The input for these parameters into a model is indicated with meteorological forcing. A more generic name for parameters that force a model is "forcing function".

Numerical solvers are applied to calculate the concentrations of substances as resulting from mass transport and water quality processes. Water quality models and the underlying numerical algorithms should be mass conserving, that is, they should not allow for the unaccounted loss or production of mass. A good water quality model should provide detailed information on mass balances.

Water quality modelling can be applied to a wide range of water quality problems. Each of those problems requires the modelling of a specific substance or group of substances. It is often necessary to include groups of state variables, if the model formulations of the individual state variables are connected to each other. For example, the decay of the state variable "organic detritus" causes the consumption of a proportional amount of the state vari-



able “dissolved oxygen”. Another example is the sedimentation of state variables representing inorganic suspended particles and adsorbed cadmium.

The table below provides an overview of common pollution problems, the associated state variables (substances), the dominant water quality processes and the main forcing functions. Note that the table is indicative only: it is not intended to be a prescription for water quality modelling.

Pollution problem	State variable(s)	Important processes	Forcing functions
Oxygen problems	Organic detritus (or BOD = biochemical oxygen demand), Dissolved oxygen	Mineralization of detritus consuming oxygen, reaeration (exchange of oxygen between water and atmosphere)	Water temperature, wind speed, stream flow velocity
Eutrophication	Algae biomass, inorganic nutrients (NH ₄ , NO ₃ , PO ₄ , Si), organic detritus	Growth and mortality of algae, mineralization of organic detritus, settling	Solar radiation, water temperature,
Heavy metal contamination	Heavy metals, inorganic suspended sediment	Partitioning-adsorption, settling, resuspension	Wind speed (flow velocity, waves)
Organic micro-pollutant contamination	Organic micro-pollutants, algae biomass, organic detritus	Partitioning, degradation, settling, resuspension	Wind speed (flow velocity, waves)
Bacterial pollution	Coliform bacteria, Escherichia coli	Mortality of bacteria	Solar radiation

A D-Water Quality model requires the following input:

- ◇ a list of substances
- ◇ the computational timestep and the time frame of the simulation
- ◇ the specification of a numerical solver
- ◇ the spatial schematization (a computational grid with cells or a set of 1D or 2D connected cells/segments)
- ◇ water flow and dispersion time series for all cells/segments
- ◇ additional dispersion coefficients (optional)
- ◇ the concentrations of all substances on the open boundaries
- ◇ the loads of substances connected to lateral discharges and “dry” loads
- ◇ a list of processes and the pertinent process coefficients
- ◇ selected forcing functions
- ◇ the initial concentrations of the state variables
- ◇ a specification of additional output parameters (optional)
- ◇ statistics of the simulated substances (optional)

Forcing functions may be meteorological, chemical, biological and hydrodynamic parameters. These functions can be time and/or space dependent. The meteorological forcing functions may include:

- ◇ the wind velocity
- ◇ the water temperature
- ◇ the solar radiation

The chemical forcing functions may include:

- ◇ the pH
- ◇ the concentrations of not simulated substances

The biological forcing functions may include:

- ◇ phytoplankton biomass
- ◇ grazer biomass

The hydrodynamic or hydraulic forcing functions may include:

- ◇ the volume;
- ◇ the horizontal surface area (from which D-Water Quality computes water depth);
- ◇ the length;
- ◇ the Chézy coefficient;
- ◇ the stream flow velocity.

When coupled to a hydrodynamics model the above time and space dependent forcing functions are automatically delivered by these models via the so-called “hyd-file” (see [section 2.2](#)).

2.1.3 The main features of the GUI

The D-Water Quality Graphical User Interface reflects the flexibility of D-Water Quality by presenting a single user interface for all D-Water Quality applications offering a similar look-and-feel for 1D, 2D and 3D models. The graphical user interface offers the following features:

- ◇ It allows easy access to most of the D-Water Quality input
- ◇ It facilitates the positioning of dry waste loads and observation points and observation areas in complex unstructured grids
- ◇ It facilitates the input of 2D spatial fields as initial conditions, horizontal dispersion or process parameters
- ◇ It facilitates the import of tabulated boundary concentrations and waste loads data
- ◇ It supports the so-called substance aliasing functionality of D-Water Quality, which is used to transfer monitored variables into modelled variables according to conversion rules
- ◇ To analyse the origin of pollutants and their path through any water system, fraction computations can be made. No additional input data is required for such computations.
- ◇ It supports sigma layer and Z-layer based vertical coordinate systems, as well as the combination of z- and sigma-layers.
- ◇ It offers full access to the D-Water Quality input file without compromising the automatic generation of parts of the input file.

2.1.4 The D-Water Quality computational core

D-Water Quality offers you some interesting features to make use of experience gained by previous users, without taking away the flexibility to build your own tailor-made water quality model. Important features of D-Water Quality are:

- ◇ D-Water Quality is based on the generic Delwaq software, which offers you more than 30 years of collective water quality modelling experience world-wide.
- ◇ D-Water Quality can simulate almost any water quality variable and the pertinent water quality processes.
- ◇ D-Water Quality is highly flexible due to the many standard and user-defined options available.
- ◇ D-Water Quality uses a library of over 600 processes and 100 substances, including salinity, nutrients, phytoplankton, vegetation, organic detritus, inorganic carbon (carbon dioxide), alkalinity, methane, dissolved oxygen, sulphur and iron components, heavy metals, organic micro-pollutants, bacterial pollutants and tracers.
- ◇ The interactive processes editor allows you to select the water quality variables and processes you want to simulate.
- ◇ Pre-defined sets of water quality variables and processes can be used for particular problems.
- ◇ Any input item can be quantified as a *constant*, a spatially varying *parameter*, a time series *function*, or a set of spatially varying time series(*segment function*).
- ◇ Concentrations of not simulated substances can be imposed to serve as input into the processes of simulated substances.
- ◇ State-of-the-art numerical schemes use a finite volume approach and provide mass balances.
- ◇ Various options are available to avoid the tedious job of defining initial and boundary conditions, loads and meteorological forcing. For example, default input can be defined for clusters of inflow locations. It is possible to overwrite defaults for specific locations, and to link your own ASCII input file with boundary data.

2.2 Schematisations & hydrodynamics

The D-Water Quality Graphical User Interface reflects the flexibility of D-Water Quality by presenting a single user interface for all D-Water Quality applications, offering a similar look-and-feel for 1D, 2D and 3D models. All information related to the model schematization and the water volumes and fluxes derived from hydrology or hydrodynamic models are organized via the so-called “hyd-file”. The hyd-file:

- ◇ contains administrative information about the schematization, the water volumes and water fluxes,
- ◇ contains references to files holding large volume data to be used by D-Water Quality.

A hyd-file with the associated bulk-data files need to be produced by a hydrology or hydrodynamics model. Presently, the following hydrodynamic models are able to produce a suitable hyd-file:

- ◇ Delft3D-FLOW;
- ◇ D-Flow Flexible Mesh;
- ◇ SOBEK-FLOW.

The hyd-file contains information as follows:

- ◇ the number of horizontal schematization elements (segments) and their shape;
- ◇ references to the files holding:

- ❑ connections between the segments (“pointer table”);
 - ❑ distances in the grid related to these connections (“lengths”)
- ◇ the locations of the model boundaries;
- ◇ the vertical grid structure (if relevant), sigma and Z-layer schematisations are supported;
- ◇ the period and interval for which data about the schematization elements and the water fluxes between them are available;
- ◇ references to the files holding data for the specified period:
 - ❑ water volumes of the segments
 - ❑ water fluxes between the segments (“flows”)
 - ❑ contact surfaces between the segments (“areas”)
 - ❑ horizontal surfaces of the segments (“surf”)
 - ❑ vertical dispersion coefficients (optional)
 - ❑ water temperature (optional)
 - ❑ salinity (optional)
 - ❑ shear stress (optional)
 - ❑ velocity (optional)
 - ❑ Chézy friction coefficient (optional)

Details are provided in [Appendix B](#).

For hydrodynamic computation using Delft3D-FM in parallel mode, the “Waqmerge” tool is used to combine the multiply output files from D-Flow FM to one single domain D-Water quality input files. Refer to the D-Water Quality Tools User Manual ([Deltares, 2024f](#)).

2.3 The Processes Library

As discussed above, depending on the problem at hand, certain substances are simulated. Apart from transport with the currents derived from the hydrodynamics model, these substances undergo various processes which are substance-specific and depend on the characteristics of the substance at hand.

D-Water Quality includes a process library from which the user can select the appropriate processes, the relevant input parameters and output quantities. This is done by means of the stand-alone Processes Library Configuration Tool (PLCT). The selections made in the PLCT are saved in so-called “sub-files” (also known as predefined sets). The D-Water Quality Graphical User Interface offers a selection of these predefined sets. Among them are a sequence of standardized water quality models copied from DUFLOW. Alternatively, the user can import a dedicated sub-file prepared with the PLCT.

The goal of the PLCT is to help the user to select the substances and the processes that act on them:

- ◇ Most substances are subjected to one or more water quality processes, for instance organic material is consumed by bacteria and with this *decay* process also dissolved oxygen is consumed. In turn this bacterial process depends on temperature: a high temperature causes it to occur faster.
- ◇ Oxygen plays a role in many processes, but in general it is not necessary to include all of them and all the substances that these processes act upon.
- ◇ The PLCT helps the user to select which substances to include in a calculation and which processes may play a role. It also helps to select the process parameters that should be varied. As process parameters usually come with a default value, you can simply rely on these values, but for some no default value is possible, for instance the solar irradiation.

While the PLCT helps in this configuration procedure, it does require some detailed knowledge of the actual water quality processes involved and of the implementation in D-Water Quality. This is also the reason for preferring the predefined sets.

Note: experienced users can add their own processes to the Processes Library and use these in addition to the available standard processes, via the so-called OpenPLCT feature.

2.4 More information

Details about the available water quality variables and processes in the Processes Library can be found in the D-Water Quality Technical Reference Manual ([Deltares, 2024e](#)).

The use of the Processes Library Configuration Tool (PLCT) is discussed in the user manual ([Deltares, 2024d](#)).

Specialist users who want to add their own variables and processes are referred to the Open-PLCT manual ([Deltares, 2024c](#)).

For a full account of the D-Water Quality input file, we refer to [Deltares \(2024b\)](#).

A mathematical description of the governing equations and the way they are solved numerically according to various numerical solvers is provided in Chapter 7.

3 D-Water Quality: Getting started

This chapter discusses the steps in the workflow of setting up a D-Water Quality model.

There are two ways to run a D-Water Quality model:

- ◇ offline coupled,
- ◇ online coupled (only available with D-Flow Flexible Mesh).

In an offline coupled model, all time steps of the hydrodynamics are computed first, followed by a water quality simulation. In an online coupled model, for each time step, both the hydrodynamics and the water quality are computed. This manual focuses on offline coupled models. For more information on online coupled models and how to set those up, the reader is referred to (Deltares, 2024a). Note that the *online* coupling is currently released as beta functionality. At this moment, this functionality is not supported in the user interface.

The workflow for an offline coupled model always starts with:

- ◇ Importing the geometry and flow data from an existing hydrodynamics model.

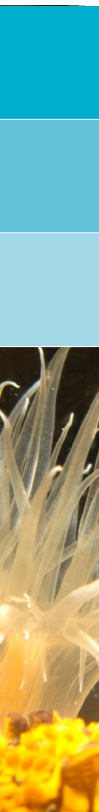
Followed by:

- ◇ Add a definition of substances and processes.
- ◇ Set initial conditions
- ◇ Set processes parameters (including meteo data)
- ◇ Set the dispersion coefficient
- ◇ Add a pollution load
- ◇ Add an observation point
- ◇ Set boundary conditions
- ◇ Set waste load data
- ◇ Run simulation
- ◇ View results

All these steps will be discussed for a small model. The focus here is on the workflow. An overview of the possibilities and options of the different steps and components is provided in the next chapter.

3.1 Starting a model

When the application Delft3D Flexible Mesh Suite or D-HYDRO Suite is started, it opens up an empty project. The first step in the modelling process is always to import an existing hydrodynamics model.



Import the geometry and flow data from an existing hydrodynamics model

Use the Import button in the ribbon

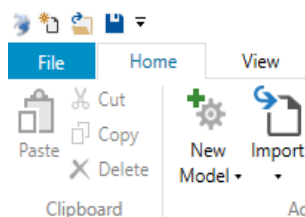


Figure 3.1: Import button in ribbon

Import a Hydrodynamics file.

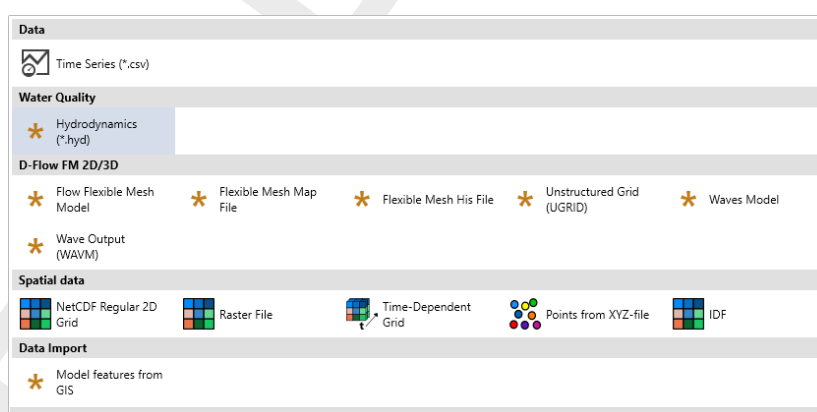


Figure 3.2: Select type of data window

The file has the extension <*.hyd>, for Delft3D-FLOW <*_unstructured.hyd>

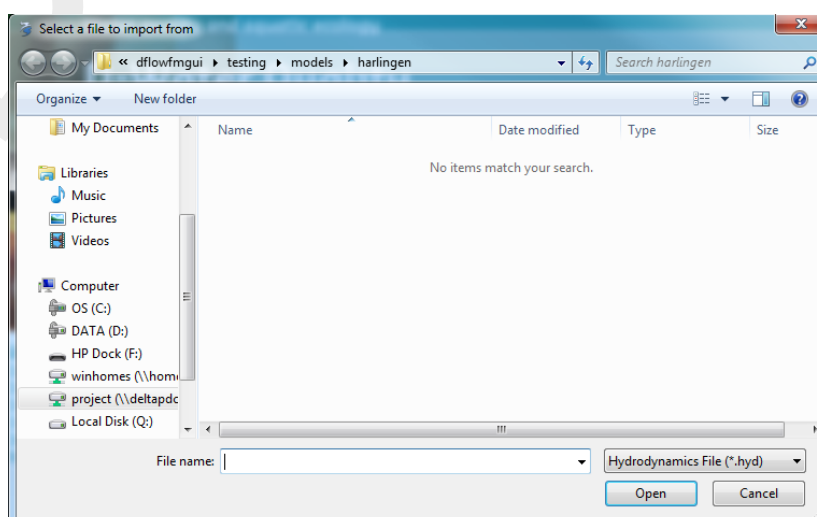


Figure 3.3: File selection window

The main window now shows the following panels:

- ◇ the project explorer (top left)

- ◇ the map explorer (bottom left)
- ◇ water quality model grid
- ◇ messages panel (bottom)
- ◇ properties panel (bottom right)

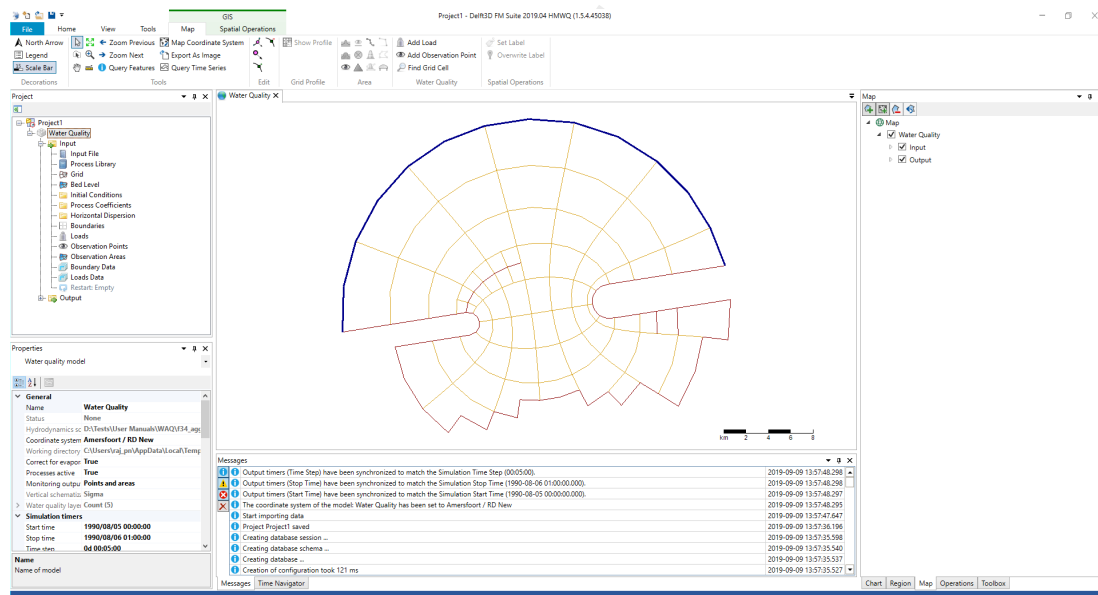


Figure 3.4: View of horizontal aggregated imported model

Note that the model grid is shown as follows:

- ◇ green lines indicate interfaces between segments (exchanges) with a flow defined
- ◇ black lines indicate closed boundaries or interfaces between segments (exchanges) without a flow
- ◇ fat blue lines indicate open boundaries (the example shown here has just one boundary called “SEA BOUNDARY”)

3.2 Setting up a fraction simulation

A fraction simulation is a simulation where different fractions of water are labelled and traced through the model domain. In this example we follow two types of water:

- ◇ “initial” water, which is present in the model domain at the start of the simulation
- ◇ “SEA BOUNDARY” water entering the model domain from the open boundary, and replacing the initial water during the simulation

Generating substances representing fractions

In the project explorer, at the item Process Library, use the right mouse button to select “Generate Fractions”. Double clicking the item Process Library allows you to inspect the results.

Name	Description	Initial value	Concentration unit
sea_002.ph	Water from boundary type sea_002.ph	0 g/h3	
sea_001.ph	Water from boundary type sea_001.ph	0 g/h3	
segsa_001.ph	Water from boundary type segsa_001.ph	0 g/h3	
yolo_001.ph	Water from boundary type yolo_001.ph	0 g/h3	
CC.ph	Water from boundary type CC.ph	0 g/h3	
tracy.ph	Water from boundary type tracy.ph	0 g/h3	
initial	Water in system at start of simulation	1 g/h3	

Name	Description	Initial value	Concentration unit
------	-------------	---------------	--------------------

Figure 3.5: Substances representing fractions

Two substances have been created, with the appropriate initial conditions.

Generating boundary conditions

In the project explorer, at the item Boundary Data, use the right mouse button to select “Generate Fraction Data”. Double clicking the item Boundary Data allows you to inspect the results.

	Name	Enabled	Data file	Substance use for file			
► 1	FractionData	<input checked="" type="checkbox"/>	FractionData.tbl	Fractions.userfor			

Data file

ITEM 'SEA BOUNDARY' CONCENTRATIONS 'SEA BOUNDARY' DATA 1

Figure 3.6: Boundary concentration for “SEA BOUNDARY”

The boundary “SEA BOUNDARY” has been given a boundary concentration for the substance “SEA BOUNDARY”, equal to 1.

Running the fraction simulation

Click on Water Quality Model in the project explorer to access the model wide properties. You can inspect and modify the simulation period, time step, output time steps, etc.

In the project explorer, at the item Water Quality Model, use the right mouse button to select “Run Model”.

You can follow the progress of the simulation in the messages panel.

After the completion of the simulation, you can inspect messages from the D-Water Quality computational program as items in the project explorer under “Output”:

- ◇ List file: <*.lst> from the input processing programme (delwaq1.exe)
- ◇ Process file: <*.lsp> from the input processing programme (delwaq1.exe)
- ◇ Monitoring file: <*.mon> from the simulation programme (delwaq2.exe)

Inspecting the results

Activate the “Initial” or “SEA BOUNDARY” output in map explorer to inspect the model output.

Activate the legend via the ribbon, to add the colour scale.

Click “Time Navigator” below the messages panel to show the Time Navigator. This will allow you to select output for specific time steps, or animate the output. The results after one tidal cycle for both fractions are shown below.

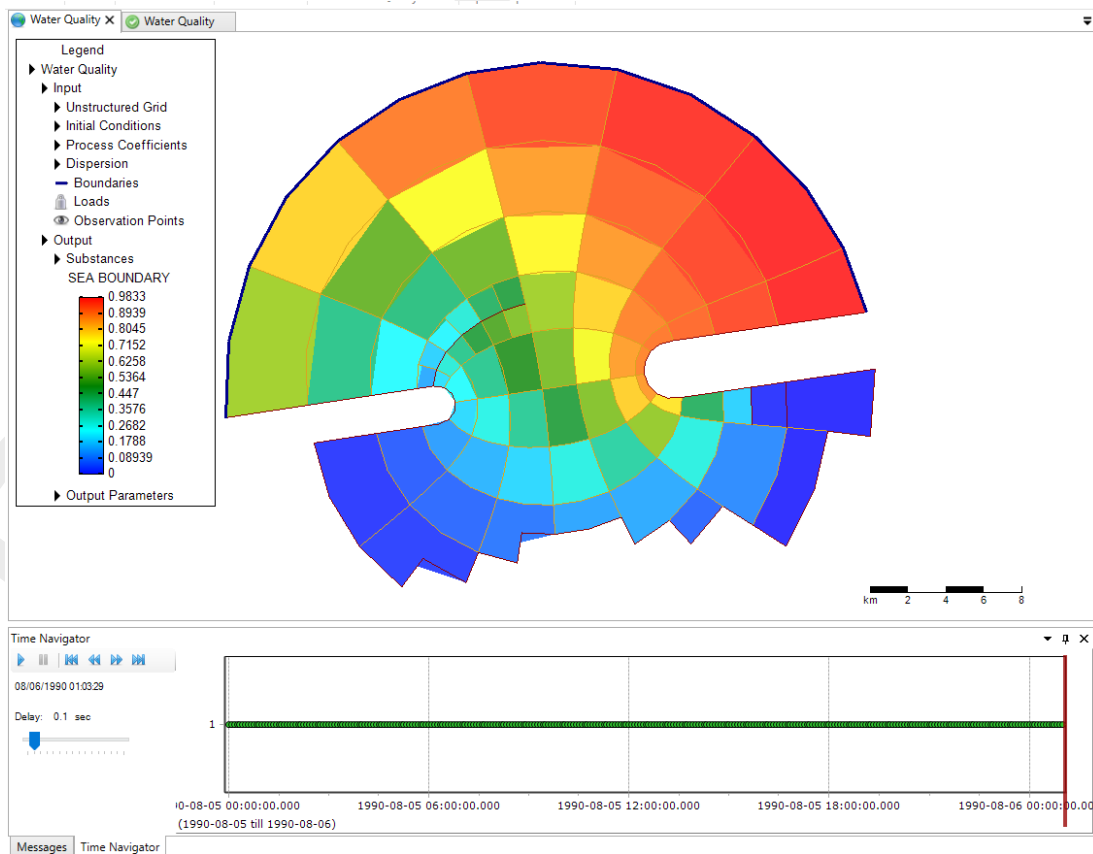


Figure 3.7: Results of “SEA BOUNDARY” after one tidal cycle

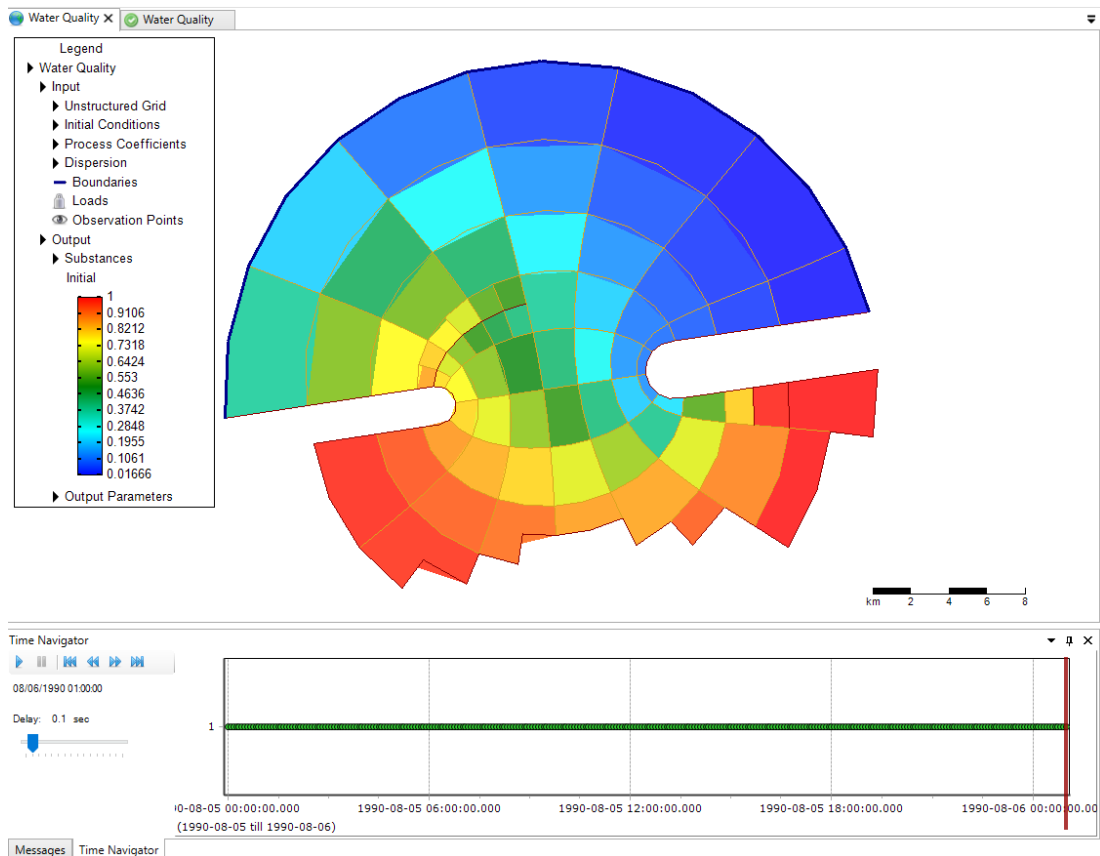


Figure 3.8: Results of initial value after one tidal cycle

3.3 Working with coordinate systems and a background map

The coordinate system of the hydrodynamics model is supposed to be included in the hyd-file you have imported. It can be inspected, and if incorrect, be changed in the properties panel of the water quality model.

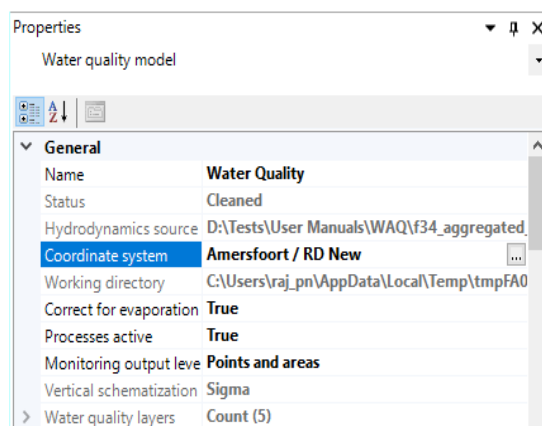


Figure 3.9: Property window



Note: Note that existing Delft3D-FLOW models always show up as Amersfoort / RD New, regardless of the real coordinate system.

Once you have set the correct coordinate system, you can show background map layers by

using the (second) Add New Wms layer button in the map panel.



Figure 3.10: Add new WMS layer

Select the appropriate web link.

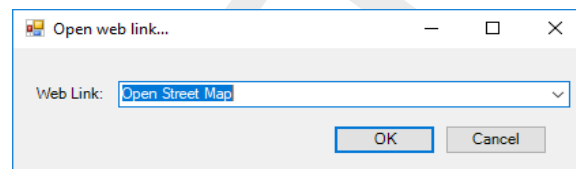


Figure 3.11: Select the appropriate WEB link

The result is as follows.

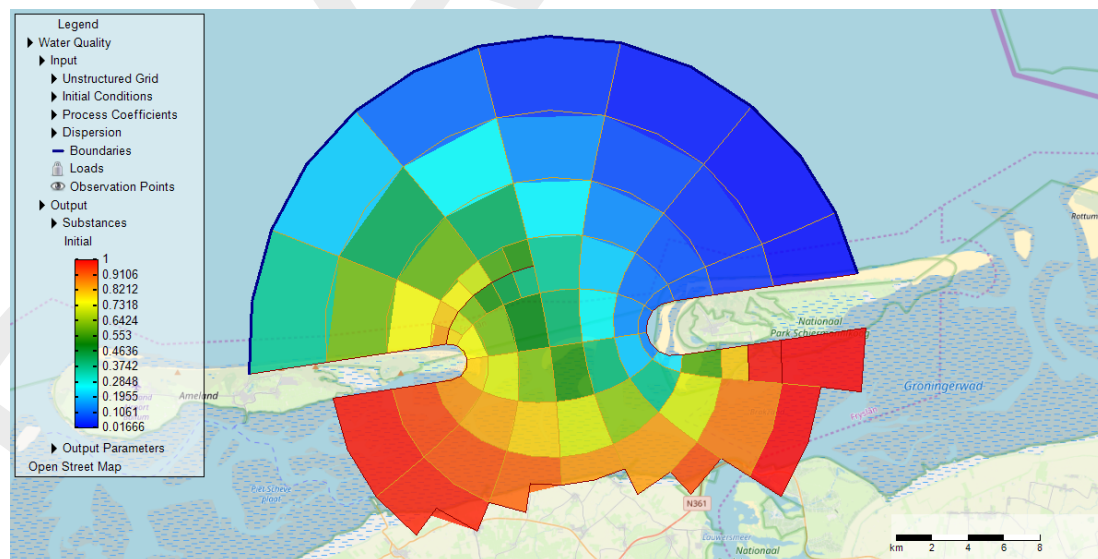


Figure 3.12: Result after selecting the WEB link

3.4 Setting up a water quality simulation

This section discusses the key steps in the workflow of setting up a D-Water Quality model. It starts after you have imported a HYD-file (see [section 3.1](#)).

Add a definition of substances and processes

The user has to make a selection from the substances and processes available in the processes library. This selection concerns:

- ◇ modelled substances
- ◇ processes
- ◇ process coefficients
- ◇ (extra) output variables

The selection is stored in a <*.sub> file. Such files can be created with the so-called PLCT utility (Processes Library Configuration Tool).

Right click on *Project/water quality model/input/process library/import*. A wizard will pop-up that guides you through the selection process.

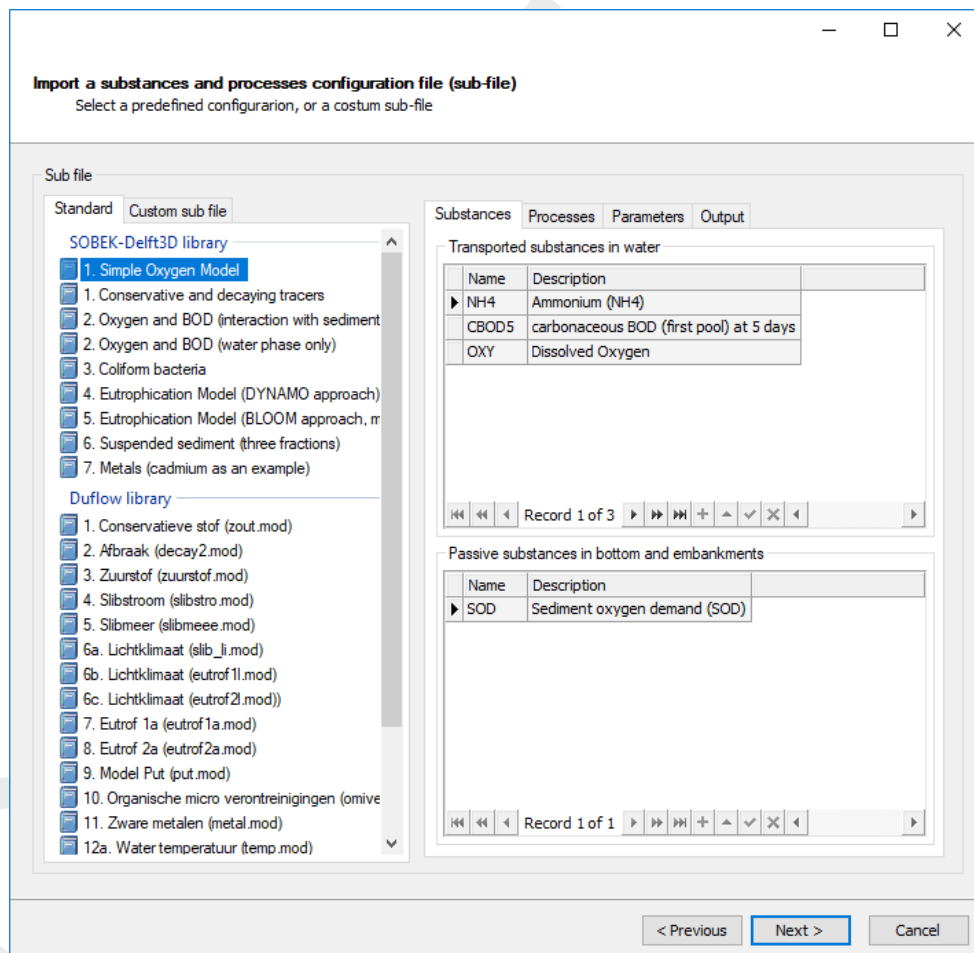


Figure 3.13: Import a substances or processes configuration file window

The Standard tab allows you to choose from a set of available sub files.

The Custom sub file tab allows you to select a sub file you have prepared yourself or copied from other users.

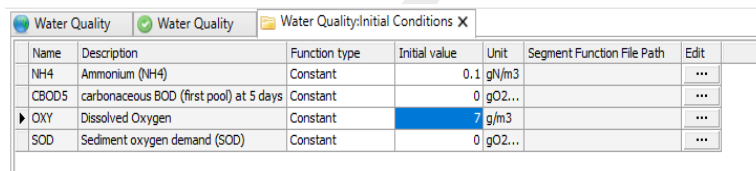
On the right side of the window, the user can screen the contents of the sub file. Several tabs will show the substances, processes, coefficients and output items which are included in the sub file.

This tutorial describes a model based on the Simple Oxygen Model.

Set initial conditions

In this example we will use homogeneous initial conditions.

You open a window to inspect and modify these values by double clicking *Project/water quality model/input/initial conditions*.

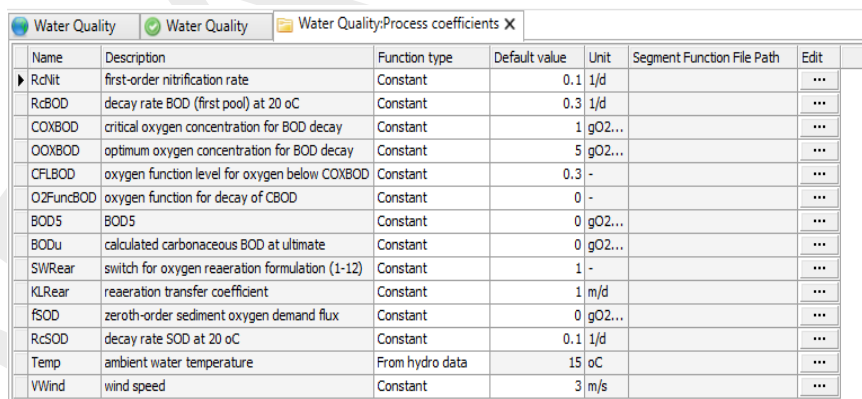


Name	Description	Function type	Initial value	Unit	Segment Function File Path	Edit
NH4	Ammonium (NH4)	Constant	0.1	gN/m3		...
CBOD5	carbonaceous BOD (first pool) at 5 days	Constant	0	gO2...		...
OXY	Dissolved Oxygen	Constant	7	g/m3		...
SOD	Sediment oxygen demand (SOD)	Constant	0	gO2...		...

Figure 3.14: Set initial values

Set processes coefficients (including meteo data)

You open a window to inspect and modify processes coefficients (including meteo data) by double clicking *Project/water quality model/input/process coefficients*.

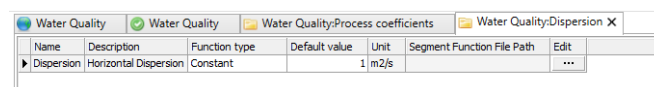


Name	Description	Function type	Default value	Unit	Segment Function File Path	Edit
RdNit	first-order nitrification rate	Constant	0.1	1/d		...
RcBOD	decay rate BOD (first pool) at 20 oC	Constant	0.3	1/d		...
COXBOD	critical oxygen concentration for BOD decay	Constant	1	gO2...		...
OOXBOD	optimum oxygen concentration for BOD decay	Constant	5	gO2...		...
CFLBOD	oxygen function level for oxygen below COXBOD	Constant	0.3	-		...
O2FuncBOD	oxygen function for decay of CBOD	Constant	0	-		...
BOD5	BOD5	Constant	0	gO2...		...
BODu	calculated carbonaceous BOD at ultimate	Constant	0	gO2...		...
SWRear	switch for oxygen reaeration formulation (1-12)	Constant	1	-		...
KLRear	reaeration transfer coefficient	Constant	1	m/d		...
fSOD	zeroth-order sediment oxygen demand flux	Constant	0	gO2...		...
RcSOD	decay rate SOD at 20 oC	Constant	0.1	1/d		...
Temp	ambient water temperature	From hydro data	15	oC		...
VWind	wind speed	Constant	3	m/s		...

Figure 3.15: Set processes coefficients

Set the dispersion coefficient

The horizontal dispersion coefficient is set by double clicking *Project/water quality model/input/horizontal dispersion*.



Name	Description	Function type	Default value	Unit	Segment Function File Path	Edit
Dispersion	Horizontal Dispersion	Constant	1	m2/s		...

Figure 3.16: Set the dispersion coefficient

The vertical dispersion coefficient is copied from the hydrodynamics model, if information to do so is passed via the hyd-file. An additional homogeneous vertical dispersion coefficient can be defined in the water quality model attributes.

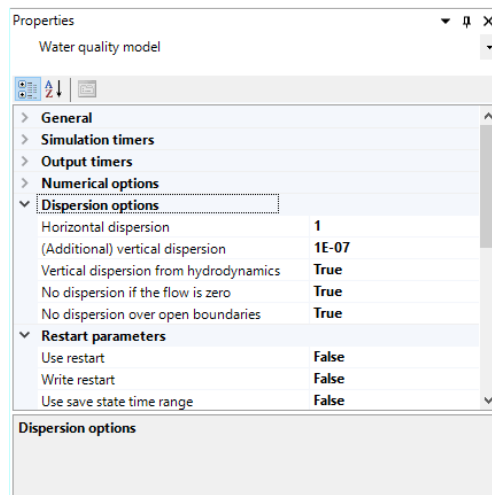




Figure 3.17: Set an additional homogeneous vertical dispersion coefficient



Add a pollution load

You define pollution loads manually from the central water quality model map. Use the  **Add Load** button on the ribbon to add a pollution load along the Frisian coast. Use the **ESC**-key or use the select  button on the ribbon to stop adding pollution loads.

The properties panel shows the name and the position of the added load, and allows you to inspect and modify these properties. Alternatively, you doubleclick *Project/water quality model/input/loads* to access a loads table. The loads will show up in the project explorer.

You can show the names of the added loads from the map explorer by right clicking *map/water quality model/input/loads/properties* and enable the labels from the labels tab.

Add observation points

You define observation points manually from the central water quality model map. Use the  **Add Observation Point** button on the ribbon to add observation points in the model domain. Use the **ESC**-key or use the select  button on the ribbon to stop adding observation points.

The properties panel shows the name and the position of the added observation point, and allows you to inspect and modify these properties. Alternatively, you doubleclick *<Project/water quality model/input/observation points>* to access an observation points table. The observation points will show up in the project explorer.

You can show the names of the added observation points from the map explorer by right clicking *map/water quality model/input/observation points/properties* and enable the labels from the labels tab.

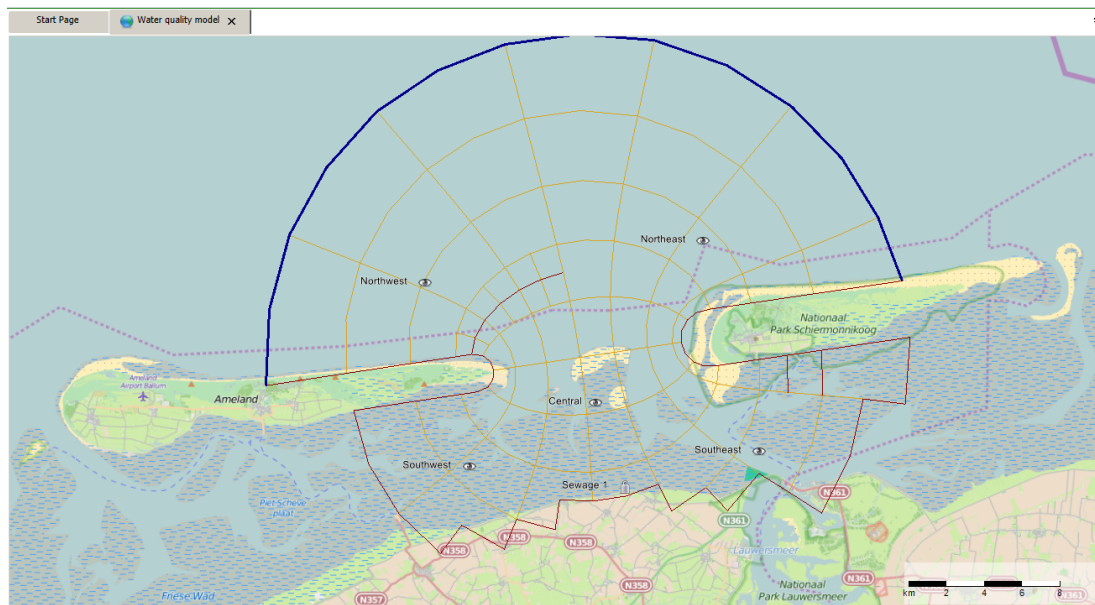


Figure 3.18: Showing the names of the added observation points

Set boundary conditions

The user interface does not contain a boundary conditions table editor, but relies on imported data only. A sample file <F34_bound.csv> is provided with the tutorial.

```
timeBlock,location,substance,value
1990-01-01 00:00:00,SEA BOUNDARY,OXY,7
1990-01-01 00:00:00,SEA BOUNDARY,NH4,0.1
```

Import this file by right clicking *Project/water quality model/input/boundary data /import*.

The result is shown below.

Name	Enabled	Data file	Substance use for file
1 F34_bound	<input checked="" type="checkbox"/>	F34_bound.tbl	F34_bound.usefors

Substances use for

USEFOR 'OXY' 'OXY'

USEFOR 'NH4' 'NH4'

Data file

```
DATA_ITEM
'SEA BOUNDARY'
CONCENTRATIONS
INCLUDE 'includes_deltashell\boundary_data_tables\F34_bound.usefors'
TIME_BLOCK DATA
'OXY' 'NH4'
1990/01/01-00:00:00 7 0.1
```

Figure 3.19: Import boundary conditions

A more detailed explanation is provided in the next chapter.

Set waste load data

The user interface does not contain a loads table editor, but relies on imported data only. A sample file <F34_load.csv> is provided with the tutorial.

```
timeBlock,location,substance,value
1990-01-01 00:00:00,Sewage 1,FLOW,0.1
1990-01-01 00:00:00,Sewage 1,CBOD5,50
```

Import this file by right clicking *Project/water quality model/input/loads data /import*.

The result is shown below.

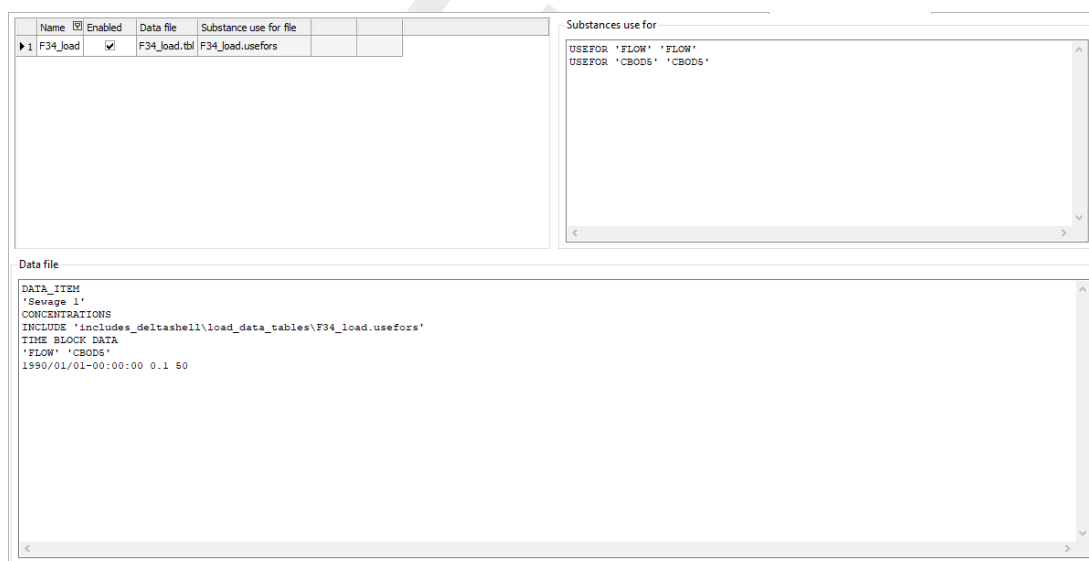


Figure 3.20: Import waste load data

A more detailed explanation is provided in the next chapter.

Run simulation

Click on Water Quality Model in the project explorer to access the model wide properties. You can inspect and modify the simulation period, time step, output time steps, etc.

In the project explorer, at the item Water Quality Model, use the right mouse button to select "Run Model".

You can follow the progress of the simulation in the messages panel.

After the completion of the simulation, you can inspect messages from the D-Water Quality computational program as items in the project explorer under "Output":

- ◇ List file: <*.lst> from the input processing programme (delwaq1.exe)
- ◇ Process file: <*.lsp> from the input processing programme (delwaq1.exe)
- ◇ Monitoring file: <*.mon> from the simulation programme (delwaq2.exe)

View results

Activate the “NH4” “CBOD5” or “OXY” output in the map explorer to inspect the model output.

Activate the legend via the ribbon, to add the colour scale.

Click “Time Navigator” below the messages panel to show the Time Navigator. This will allow you to select output for specific time steps, or animate the output.

Time series output can be visualised by right clicking on a segment in the map. This time series output will have the output interval specified under the Model wide (map) output timers in the properties panel.

For observation points you can visualise time series output by double clicking an observation point in the project explorer. This time series output will have the output interval specified under the Observation points and areas (his) output timers in the properties panel.

DRAFT

4 D-Water Quality: All about the modelling process

This chapter discusses the details of the functionality of the user interface. It follows the basic steps in the workflow of setting up a D-Water Quality model. Before you read this chapter, please go through the basic workflow steps discussed in [chapter 3](#).

This chapter provides certain details which are only familiar to experienced users. We provide them for the sake of completeness. Less experienced users can ignore such remarks.

4.1 Starting a model and Importing the geometry and flow data from an existing hydrodynamics model

Importing geometry and flow data from an existing hydrodynamics model is always the first step of the modelling process. This information is accessed via a so-called `<*.hyd>` file (or hyd-file). This file is actually an administrative file that provides basic information and refers to other relevant files containing essential or optional information (see [Appendix B](#) for a formal description). The hyd-file used by the D-Water Quality GUI is independent of the kind of hydrodynamics model: 1D or 2D/3D, structured or unstructured.

4.1.1 Grid definition

A D-Water Quality model consists of so-called segments. After the import, the GUI will show you these segments on the map.

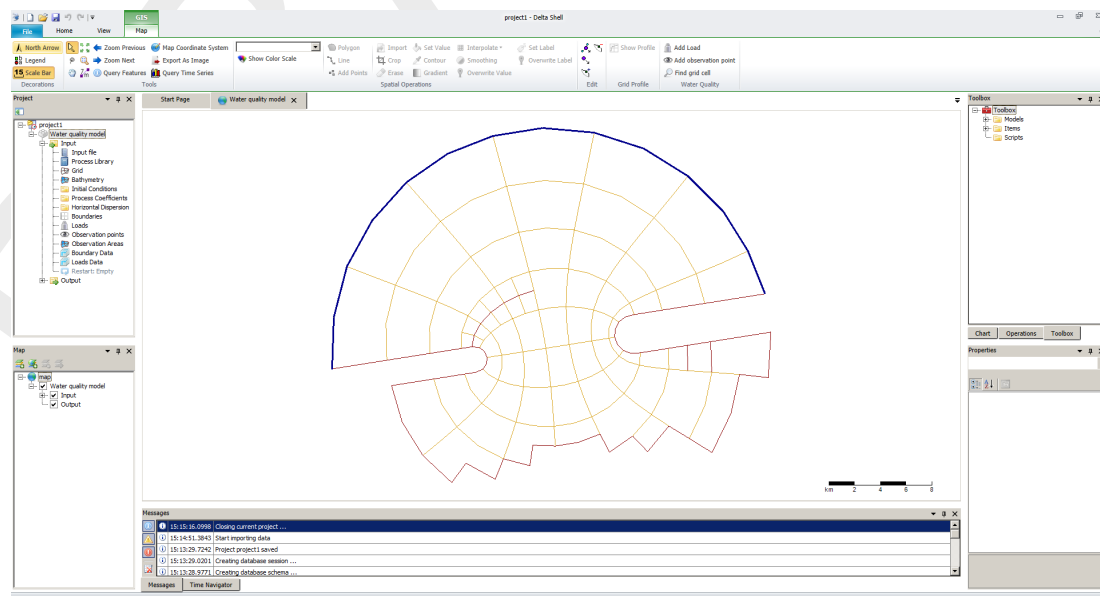
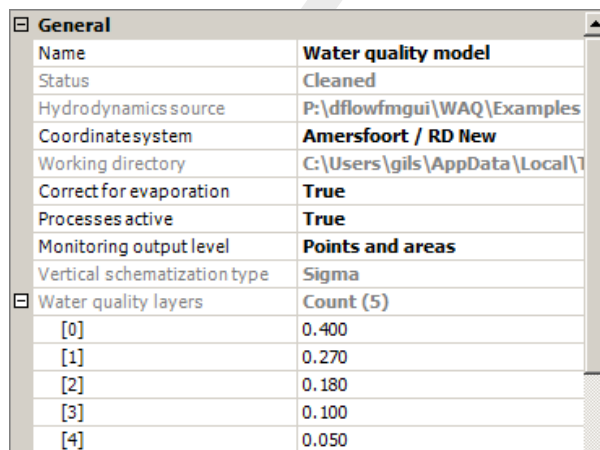


Figure 4.1: D-Water Quality grid definition

If you have a 3D model, the hyd-file provides information about the vertical grid structure as well. There are two options: a sigma layer model or a Z layer model

Sigma layers

Every horizontal segment actually consists of a constant number of vertical layers. Each layer covers a fixed fraction of the total water column. This implies that the actual thickness of each layer varies with the water level. The number of layers and their relative thickness can be inspected under the water quality model properties (right click *Project/water quality model/properties*).



General	
Name	Water quality model
Status	Cleaned
Hydrodynamics source	P:\dflowmgui\WAQ\Examples
Coordinates system	Amersfoort / RD New
Working directory	C:\Users\gils\AppData\Local\T
Correct for evaporation	True
Processes active	True
Monitoring output level	Points and areas
Vertical schematization type	Sigma
Water quality layers	Count (5)
[0]	0.400
[1]	0.270
[2]	0.180
[3]	0.100
[4]	0.050

Figure 4.2: General parameters, σ -layer model

The vertical coordinate σ is a relative coordinate and runs from:

- ◇ $\sigma = 0$ at the water surface to
- ◇ $\sigma = 1$ at the water sediment interface

Z layers

In the grid administration, every horizontal segment consists of a fixed number of vertical layers. The interfaces between the layers are defined at a fixed absolute vertical coordinate. This implies that the thickness of all layers is constant, unless the water surface happens to be in that layer. In that case the actual water level determines the layer thickness. In the layer where the water level is, the thickness varies with time and space.

The position of the bed determines how many of the defined layers actually contain water. Also, the layer where the bed is, is thinner in reality than its defined thickness.

The vertical coordinate z is an absolute coordinate, which increases in an upward direction. The values are determined by the hydrodynamics layers vertical coordinates. In particular:

- ◇ z -top = at the top of the upper layer
- ◇ z -bot = at the bottom of the lower layer.

4.1.2 Segment properties

The hyd-file provides the following information about these segments:

- ◇ outline (see above) (compulsory)
- ◇ two so-called attributes (see [Deltares \(2024b, section 3.7\)](#)) (compulsory)
- ◇ time dependent volume (m^3 , compulsory)
- ◇ horizontal surface area, optionally time dependent (m^2 , compulsory)
- ◇ time dependent salinity (ppt, optional)

- ◇ time dependent temperature ($^{\circ}\text{C}$, optional)
- ◇ time dependent shear stress (Pa, optional)
- ◇ time dependent Chézy coefficient ($\text{m}^{1/2}/\text{s}$, optional)
- ◇ time dependent velocity (m/s, optional)

The optional items are all quantities which can be calculated by a hydrodynamics model and can be input to specific water quality processes. If they are required by the selected processes, and if the hyd-file provides them, the GUI will automatically pass them to the computational core.

The horizontal surface area is typically constant in a 2D or 3D model. In a 1D model it can vary with time, because such models often account for an increasing branch width with increasing water level.

4.1.3 Exchanges and exchanges properties

D-Water Quality simulates the transport of pollutants in water bodies by using exchanges between segments. An exchange is defined by information derived from the hyd-file:

- ◇ a “from segment” or “from boundary” (compulsory)
- ◇ a “to segment” or “to boundary” (compulsory)
- ◇ discharge (m^3/s , compulsory)
- ◇ area of contact between two connected segments (m^2 , compulsory)
- ◇ distance to centre of “from segment” (m, compulsory)
- ◇ distance to centre of “to segment” (m, compulsory)
- ◇ dispersion coefficient (m^2/s , optional, only vertical)

Note: Note that the model grid as shown by the GUI also reveals the exchanges:



- ◇ green lines indicate interfaces between segments where an exchanges is defined
- ◇ black lines indicate closed boundaries or interfaces between segments where NO exchange is defined (for example a so-called “thin dam”)
- ◇ fat blue lines indicate open boundaries, where an exchange is defined

4.1.4 Vertical dispersion

Vertical dispersion is determined by the vertical turbulence structure which is strongly affected by vertical temperature and salinity gradients. Such gradients are typically calculated by 3D hydrodynamic models and this also holds for the vertical dispersion coefficient. Therefore, the vertical dispersion coefficient can optionally be derived from the hydrodynamics model via the hyd-file.

4.1.5 Time frames

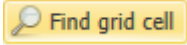

The hyd-file provides time dependent data from the hydrodynamics model for a defined period and with a defined time interval. Because some file formats for time dependent data use a relative time indicator, the absolute reference date and time is also derived from the hyd-file, and copied to D-Water Quality’s so-called “T0 string” (see [Deltares \(2024b\)](#), Section 1.3)).

4.1.6 Available links to hydrodynamics models

The present definition of the hyd-file is supported by:

- ◇ D-Flow FM, sigma layers only ([Deltares, 2024a](#)).
- ◇ Delft3D-FLOW, from version 4.0.2 onwards (use file <*_unstructured.hyd>)
- ◇ SOBEK-FLOW (see [Deltares \(2015\)](#))

4.1.7 Finding a particular segment

Use the  button on the ribbon to search for a specific grid cell. The GUI will colour the relevant cell, and indicate the layer number in the map window. Use the `ESC`-key or use the select  button on the ribbon to stop showing the selected segment.

4.2 The D-Water Quality input file

As a user you have full access to the D-Water Quality Input file. The default version of that file is embedded in every new model you create. It is accessible by double clicking *project/water quality model/input file*.

```
1000 80 ','
;DELWAQ_VERSION 4.910                ; Delwaq version number
;PRINT_OUTPUT_OPTION_4              ; Debug level

; TEMPLATE FILE FOR WATER QUALITY CALCULATION
; First input block
'Water quality calculation'
' '
' '
INCLUDE 'includes_deltashell\B1_t0.inc'      ; From UI: Time stamp
INCLUDE 'includes_deltashell\B1_sublist.inc' ; From UI: Substance list
#1;

;#####
; Second input block
86400 'DDHHMMSS' 'DDHHMMSS'                ; system clock
INCLUDE 'includes_deltashell\B2_numsettings.inc' ; From UI: Simulation timers
INCLUDE 'includes_deltashell\B2_simtimers.inc'  ; From UI: Simulation timers
1                                              ; Monitoring areas in this file
INCLUDE 'includes_deltashell\B2_outlocs.inc'    ; From UI: Definition of output locations
2                                              ; No monitoring cross areas
INCLUDE 'includes_deltashell\B2_outputtimers.inc' ; From UI: Simulation timers
#2;

;#####
; Third input block
INCLUDE 'includes_deltashell\B3_nrofseg.inc'    ; From UI: Nr of segments (multiply number-water-quality-segments-per-layer
and number-water-quality-layers from HYD)
2                                              ; Structure matrix not used
INCLUDE 'includes_deltashell\B3_attributes.inc' ; From UI: attributes file
INCLUDE 'includes_deltashell\B3_volumes.inc'   ; From UI: volumes-file
#3;
;#####
```

Figure 4.3: View on D-Water Quality input file

In the input file, you will see that certain files created by the GUI are included, e.g. the file <includes_deltashell\B1_t0.inc> that holds the T0 string.

Changing the input file

You are free to change the input file. Your changes will be saved as part of the model. Thus, you can add features not supported by the GUI to your input file, or you can create quick workarounds for erroneous features of the GUI. It is needless to say that such changes should only be done with care and by expert users.



Note: If you include your own files by editing the input file, make sure to store these files OUTSIDE the model folders that the GUI creates (see [section 4.17](#)).

Restoring the default input file

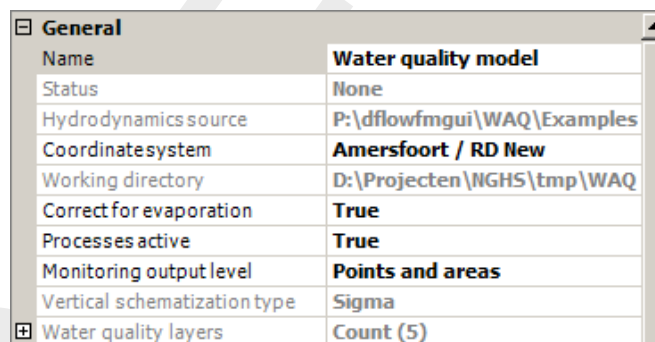
You can always revert to the original version of the input file by creating a new model. In an existing model, right click on *project/water quality model/input file/revert to original template*.

Formal description of the input file

For a full description, we refer to the [Deltares \(2024b\)](#).

4.3 General water quality model properties

After importing a hyd-file, some general model properties are set. Inspect them by a right click on *project/water quality model*. The properties you can change are printed in **bold**.



General	
Name	Water quality model
Status	None
Hydrodynamics source	P:\dflowmgui\WAQ\Examples
Coordinatesystem	Amersfoort / RD New
Working directory	D:\Projecten\NGHS\tmp\WAQ
Correct for evaporation	True
Processes active	True
Monitoring output level	Points and areas
Vertical schematization type	Sigma
Water quality layers	Count (5)

Figure 4.4: General water quality model properties

Name

Here you can change the name of the model.

Coordinate system

The GUI operates in a defined coordinate system. The coordinate system is supposed to be included in the hyd-file you have imported. It can be inspected, and if incorrect, be changed here.

Processes active

Here you can choose to activate all processes from the processes library or not. As a rule you run with processes active. Running without processes could be useful during troubleshooting.

Note: This is equivalent to the `delwaq1 --p` and `--np` command line switches.

Note: Running without processes will also remove vertical dispersion derived from the hydrodynamics model and spatially varying horizontal dispersion.



Monitoring output level

The GUI supports the definition of observation points and observation areas. Here you can select if you want to write output for these observation points and areas.

4.4 Simulation and Output timers

You access the timers of your simulation in the properties panel by a right click on *project/water quality model*. After loading a hyd-file for the first time, all timers are made equal to the period and interval for which the hyd-file provides data.

<input checked="" type="checkbox"/> Simulation timers	
Start time	1990-08-05 00:00:00
Stop time	1990-08-06 01:00:00
Time step	0d 00:05:00
<input checked="" type="checkbox"/> Output timers	
<input checked="" type="checkbox"/> Observation points and areas (f)	
Start time	1990-08-05 00:00:00
Stop time	1990-08-06 01:00:00
Time step	0d 00:05:00
<input checked="" type="checkbox"/> Model wide (map)	
Start time	1990-08-05 00:00:00
Stop time	1990-08-06 01:00:00
Time step	0d 00:05:00
<input checked="" type="checkbox"/> Balances (mon)	
Start time	1990-08-05 00:00:00
Stop time	1990-08-06 01:00:00
Time step	0d 00:05:00

Figure 4.5: Simulation and Output timers

Simulation timers

The start of your simulation should always be on or after the start of the hyd-file data. The end of your simulation can be chosen freely. As soon as you pass the stop time of the hyd-file data, the computational core will repeat the hyd-file data, as often as necessary to reach the requested end time of the simulation. In such cases, you may choose to activate the closure error correction (see [Numerical options](#)).

Your simulation time step should not exceed the time interval in the hyd-file. The computational core does not have the ability to integrate water flow information provided via the hyd-file. If you choose your time step larger than the time interval in the hyd-file, certain records in the water flow file will be skipped, and this will compromise the validity of the water balance provided via the hyd-file.

Output timers

Output can be requested for any period with any time step. Evidently, the output you can obtain will be limited to the available simulation period and simulation time step. Note that different types of output can be written for different periods and with different time intervals, to manage the size of your output files.

4.5 Numerical options

You access the numerical options in the properties panel by a right click on *project/water quality model*.

Numerical options	
Integration method	Scheme 15
Use first order open boundary t	False
Max nr of iterations	100
Iteration convergence criterion	1E-07
Iteration report	False
Closure error correction	True
Dry cell threshold (m)	0.001
Nr of cores to use (0 = max)	0

Figure 4.6: Numerical options

Integration Method

D-Water Quality offers a sequence of numerical methods to solve the transport terms (advection and dispersion) of the governing equations. For a description of the full range of available methods, we refer to the [Deltares \(2024g, Section 10\)](#). Here, we briefly mention the most common methods:

- ◇ Scheme 15, an Implicit Upwind scheme with an iterative solver, provides unconditional stability, but is not very good in reproducing sharp concentration gradients in space and/or time.
- ◇ Scheme 5 (for 1D / 2D models) or scheme 12 (3D models), provide second-order (high) accuracy in all horizontal directions. In the horizontal direction however, these schemes are subject to the so-called Courant-Friedrichs-Lewy (CFL) stability criterion, which can be expressed as follows: the volume of water replaced within any grid cell within one time step must always be smaller than the volume of the grid cell. Depending on the hydrodynamics model results and the optional aggregation of such results, this condition may lead to a very small time step.
- ◇ Scheme 22 offers a blend of the two schemes mentioned above. Where and when possible scheme 12 is used, otherwise scheme 15. Research has indicated that this approach effectively alleviates the stability problems of schemes 5/12 while maintaining a substantially higher accuracy than scheme 15.
- ◇ Scheme 24 is a modified version of scheme 12 and avoids stability problems by automatic selective time step reduction.

We note that water quality processes and loads are always included *explicitly* in the integration of the governing equations. This implies that processes representing a sink and negative loads (withdrawals) will be subject to a stability criterion: you cannot remove more mass per time step than the amount of mass present at the beginning of the time step. For a linear decay process a necessary condition is $\Delta t < 1/k$, where Δt is the time step [s] and k is the first-order decay rate [s]. For a withdrawal of Q [m^3/s] from a segment with a volume V [m^3], a necessary condition is $\Delta t < V/Q$. In reality, such stability criteria may be stricter because of other processes also removing mass.

Use first-order open boundary transport

This option is relevant for second-order schemes. We recommend to use it. It forces a first-order transport discretization over open boundaries. This implies that over open boundaries having an inflow of water, the transport equals the water flow [m^3/s] multiplied with the boundary concentration [g/m^3] which is what we intuitively assume.

Iteration control

For schemes using the iterative implicit solver (15/16/21/22), the iteration process can be controlled. The iteration convergence criterion determines the maximum allowable deviation between the numerical solution and the real solution. The default value of 10^{-7} has been chosen as an acceptable value in many practical cases. Higher values, allowing larger deviations between the numerical solution and the real solution, should only be applied with great care. We have encountered practical cases where the criterion needed to be tightened to 10^{-12} to obtain an accurate solution. Insufficient accuracy can be recognized sometimes from unrealistic results. An objective measure can be obtained from the mass balances output. The Max nr of iterations should be high enough to obtain the requested accuracy of the iteration process. If this is not the case, an error will result:

```
ERROR in GMRES 1 1
Solver did not reach convergence
```

Such an error should be resolved by increasing the number of iterations, and only with great care by releasing the convergence criterion. There are cases when the convergence is so slow, that simulation times will reach unacceptable levels. A common cause for this is a dominance of dispersion over advection. If this is an essential feature of your model, schemes using the iterative implicit solver will not be of use for you. 3D tidal models however, can usually do very well without dispersion, and you may consider not to use dispersion in order to enhance convergence.

Closure error correction

If you repeat the hyd-file data, there will be a discontinuity in the water levels if you jump from the last time in the hyd-file to the first time. This will result in a jump of the volume of the segments. Because D-Water Quality's primary state variable is mass, a volume jump will result in a concentration jump. Applying the closure error correction will avoid such a jump by correcting the mass proportional to the volume jump. For more details we refer to [Deltares \(2024b, Section 7.3.1.1\)](#). We note that this correction compromises the mass balance. We also note that this correction is not yet visible in the mass balances output. It will show up as a mass error.

Dry cell threshold

Here you can set the special constant DRY_THRESH (unit m), which plays a role in the handling of drying and flooding. For more details we refer to [Deltares \(2024b, Section 7.3.1.1\)](#).

Number of cores to use

Using multiple cores allows you to benefit from D-Water Quality's parallelisation features. Here you can set the number of cores D-Water Quality should use. A value of 0 will result in the use of all cores. Using a reduced number of cores will allow you to keep working on your computer while D-Water Quality is running.

4.6 Add a definition of substances and processes

The selection of a set of substances and processes by selecting a sub file has been discussed under “Getting started”.

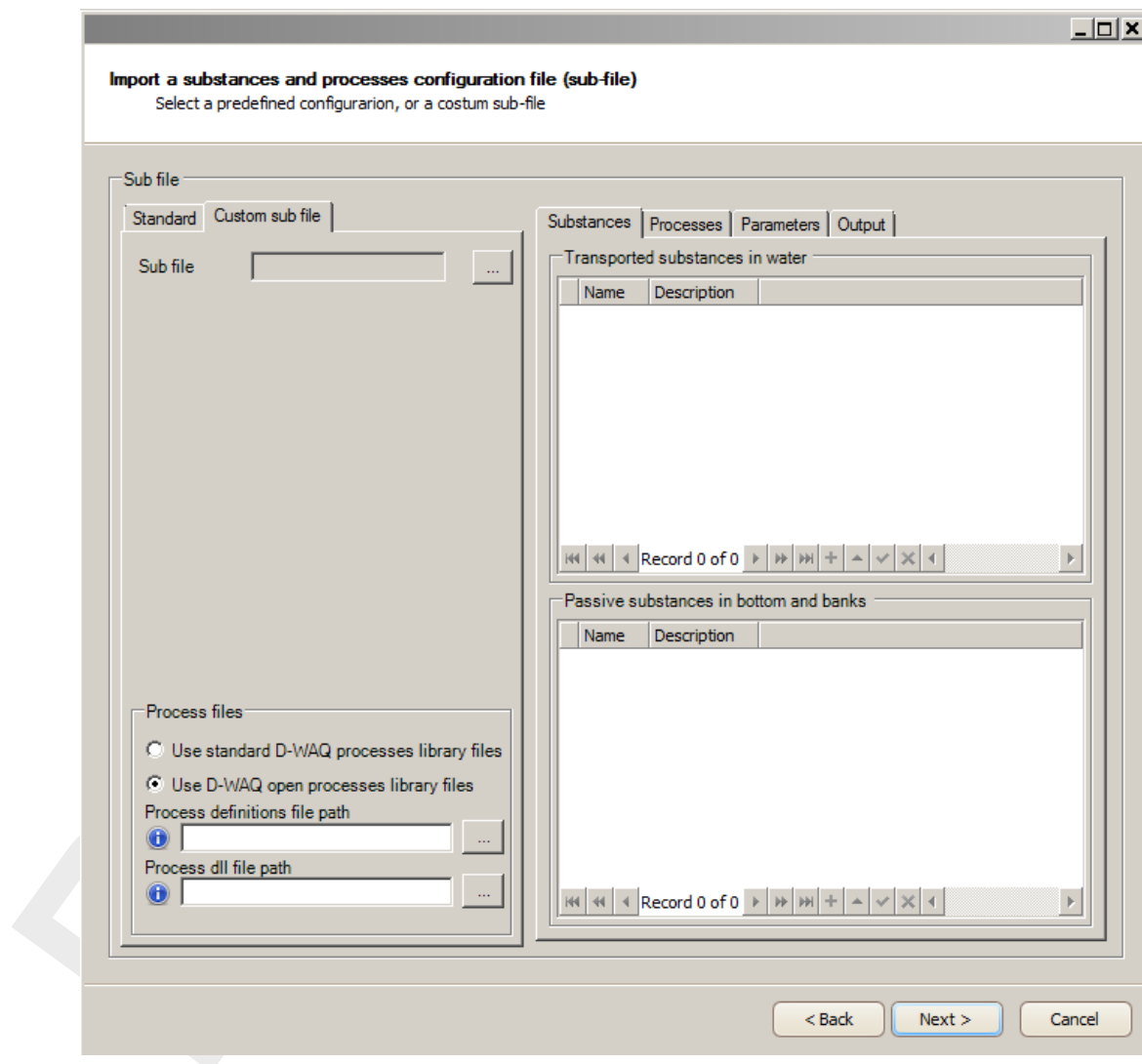


Figure 4.7: Substances file import wizard

4.6.1 The PLCT (Processes Library Configuration Tool)

You create a sub file with the PLCT (Processes Library Configuration Tool). This tool has been installed as a stand alone application in the Windows Start menu in the Delt3D FM folder. The manual for the PLCT explains in detail how to use it (Deltares, 2024d).

The import wizard for the sub files within the D-Water Quality GUI allows you to choose a custom sub file created via the PLCT.

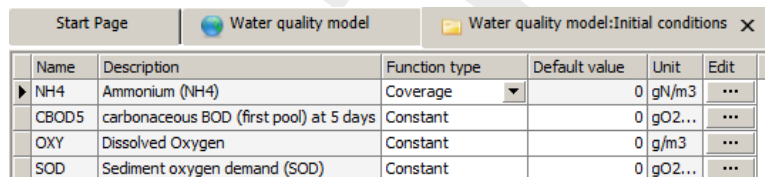
Note for advanced users: If you use your own processes library (see Deltares (2024c)), then you need to specify the processes DLL that holds the compiled program code of your extra processes and the dedicated process definition file (<proc_def.def> and <proc_def.dat>), consisting of the definitions of the standard processes included in D-Water Quality plus the definitions of the extra processes.

4.7 Set initial conditions

For working with homogeneous initial conditions we refer to [chapter 3](#). Here, we discuss more elaborate options.

4.7.1 Spatial fields

For setting spatially variable initial conditions, you open the initial conditions table by double clicking *Project/water quality model/input/initial conditions*. In the function type column you make the initial condition a “Coverage” if you want to define a spatial field.



Name	Description	Function type	Default value	Unit	Edit
NH4	Ammonium (NH4)	Coverage	0	gN/m3	...
CBOD5	carbonaceous BOD (first pool) at 5 days	Constant	0	gO2...	...
OXY	Dissolved Oxygen	Constant	0	g/m3	...
SOD	Sediment oxygen demand (SOD)	Constant	0	gO2...	...

Figure 4.8: Spatial fields



Note: Note that a spatially variable initial condition is indicated in the project explorer.

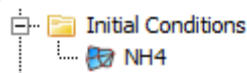


Figure 4.9: Indication in project explorer of initial conditions for NH₄

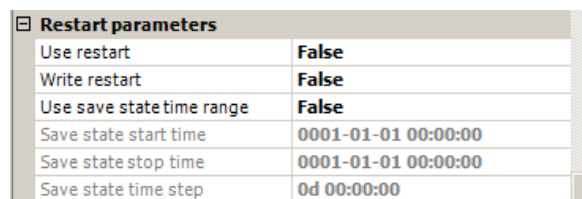
By clicking in the Edit column you activate the Spatial Editor. You can:

- ◇ build a spatial field by drawing polygons and allocating values to those polygons, followed by various spatial operations like interpolation;
- ◇ building a spatial field on the basis of an imported set of samples.

For defining a spatial field with the Spatial Editor we refer to the [Deltares \(2024i, section 5\)](#).

Note that the present version of the Spatial Editor only supports two-dimensional spatial fields. If your model is 3D, the WAQ GUI will create vertically homogeneous initial conditions.

4.7.2 Restarting



Restart parameters	
Use restart	False
Write restart	False
Use save state time range	False
Save state start time	0001-01-01 00:00:00
Save state stop time	0001-01-01 00:00:00
Save state time step	0d 00:00:00

Figure 4.10: Restart parameters

4.8 Set process coefficients (including meteo data)

For working with constant process coefficients we refer to [chapter 3](#). Here, we discuss more elaborate options.

4.8.1 Time functions

For setting time dependent process coefficients, you open the process coefficients table by double clicking *Project/water quality model/input/ process coefficients*. In the function type column you make the process coefficient a “Time Series” if you want to define a time function.

Start Page		Water quality model		Water quality model:Process coefficients		
Name	Description	Function type	Default value	Unit	Edit	
RdNit	first-order nitrification rate	Constant	0.1	1/d	...	
RcBOD	decay rate BOD (first pool) at 20 oC	Constant	0.3	1/d	...	
COXBOD	critical oxygen concentration for BOD decay	Constant	1	gO2...	...	
OOXBOD	optimum oxygen concentration for BOD decay	Constant	5	gO2...	...	
CFLBOD	oxygen function level for oxygen below COXBOD	Constant	0.3	-	...	
O2FuncBOD	oxygen function for decay of CBOD	Constant	0	-	...	
BOD5	BOD5	Constant	0	gO2...	...	
BODu	calculated carbonaceous BOD at ultimate	Constant	0	gO2...	...	
SWRear	switch for oxygen reaeration formulation (1-12)	Constant	1	-	...	
KLear	reaeration transfer coefficient	Constant	1	m/d	...	
fSOD	zeroth-order sediment oxygen demand flux	Coverage	0	gO2...	...	
RcSOD	decay rate SOD at 20 oC	Constant	0.1	1/d	...	
Temp	ambient water temperature	From hydro data	15	oC	...	
VWind	wind speed	Time series	3	m/s	...	

Figure 4.11: Time functions

Note: Note that a time dependent process coefficient is indicated in the project explorer.



Figure 4.12: Indication in project explorer of process coefficients *fSOD* and *VWIND*

By clicking in the *Edit* column you activate the Time Series Editor. This editor allows you to define and inspect time series. A clipboard and csv-import function is available.

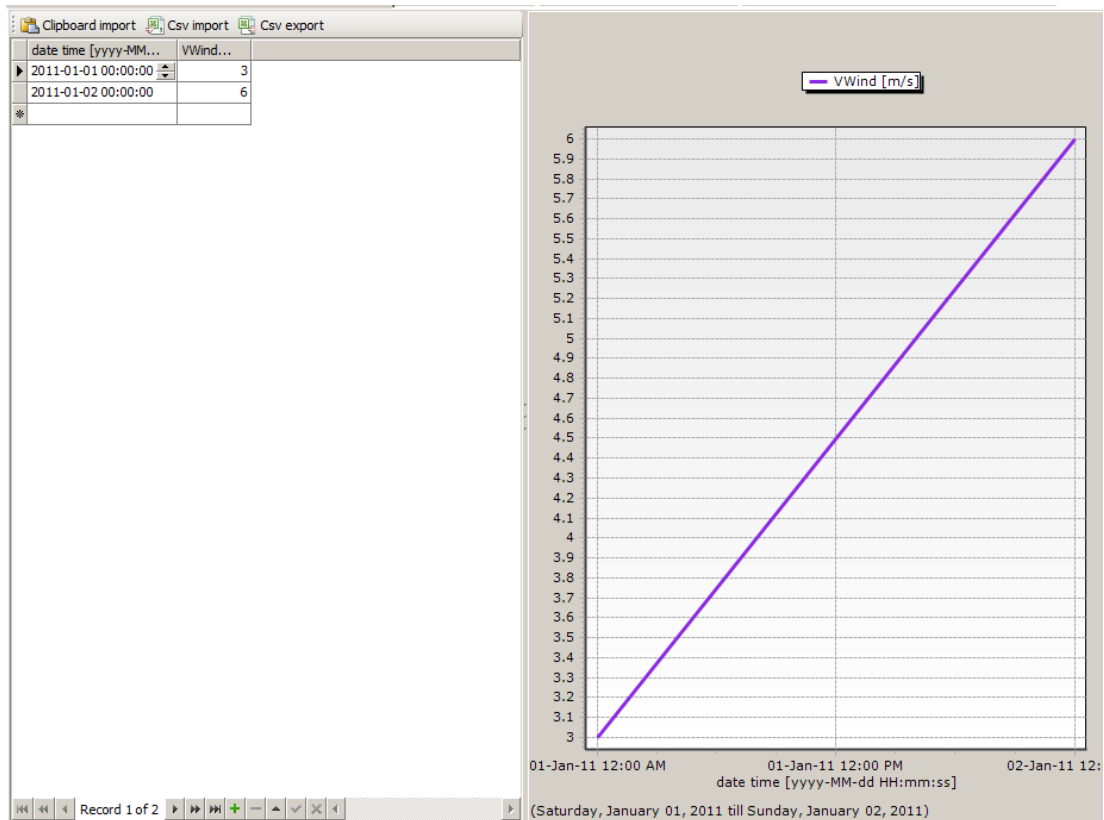


Figure 4.13: Time series editor

4.8.2 Spatial fields

For setting spatially variable process coefficients, you open the process coefficients table by double clicking *Project/water quality model/input/ process coefficients*. In the function type column you make the process coefficient a “Coverage” if you want to define a spatial field.





Start Page		 Water quality model		 Water quality model:Process coefficients 	
Name	Description	Function type	Default value	Unit	Edit
► RcNit	first-order nitrification rate	Constant 	0.1	1/d	...
RcBOD	decay rate BOD (first pool) at 20 oC	Constant	0.3	1/d	...
COXBOD	critical oxygen concentration for BOD decay	Constant	1	gO2...	...
OOXBOD	optimum oxygen concentration for BOD decay	Constant	5	gO2...	...
CFLBOD	oxygen function level for oxygen below COXBOD	Constant	0.3	-	...
O2FuncBOD	oxygen function for decay of CBOD	Constant	0	-	...
BOD5	BOD5	Constant	0	gO2...	...
BODu	calculated carbonaceous BOD at ultimate	Constant	0	gO2...	...
SWRear	switch for oxygen reaeration formulation (1-12)	Constant	1	-	...
KLRear	reaeration transfer coefficient	Constant	1	m/d	...
fSOD	zeroth-order sediment oxygen demand flux	Coverage	0	gO2...	...
RcSOD	decay rate SOD at 20 oC	Constant	0.1	1/d	...
Temp	ambient water temperature	From hydro data	15	oC	...
VWind	wind speed	Time series	3	m/s	...

Figure 4.14: Spatial fields



Note: Note that a time dependent process coefficient is indicated in the project explorer.



Figure 4.15: Indication in project explorer of time dependent process coefficient VWIND

By clicking in the *Edit* column you activate the Spatial Editor. See the Initial Conditions section for more details.

Note: Note that the present version of the Spatial Editor only supports two-dimensional spatial fields. If your model is 3D, the WAQ GUI will create vertically homogeneous process coefficients.



4.8.3 Link to hydro data

If one or more of the process coefficients are available from the hyd-file, the WAQ GUI will automatically pass this information to D-Water Quality. In the process coefficients table you will see such a coefficient indicated as “From hydro data” in the function type column.

4.8.4 Coefficients for the BLOOM algae sub model

There is a dedicated tabular parameter editor available for the editing of BLOOM parameters, which is only visible when BLOOM parameters are present in the substance file.

BLOOM Algae Type	EXTVL[ALG]	NCR[...]	PCR[ALG]	SCR[ALG]	CHLAC[ALG]	DMCF[ALG]	PPMAX[ALG]	MORT[ALG]	TCMRT[ALG]	MRESP[ALG]	TCRSP[ALG]	SOMD[ALG]	VOSed[Alg]	FrAut[Alg]	FrDet[Alg]	n[Alg]	Fr[Alg]
FDL_P (Fresh DIATOMS P/Si type)	0.1875	0.188	0.0113	0.55	0.025	2.5	0.35	0.045	1.085	0.031	1.072	1	0	0.35	0.55	0	0
BLU_E (BLUEGRN energy type)	0.4	0.225	0.0188	0.0018	0.033	2.5	0.056	0.035	1.08	0.012	1.072	1	0	0.35	0.62	0	0
GRE_N (GREENS nitrogen type)	0.1875	0.175	0.015	0.0018	0.025	2.5	0.068	0.045	1.085	0.031	1.072	1	0	0.35	0.55	0	0
GRE_P (GREENS phosphorus type)	0.1875	0.15	0.0125	0.0018	0.025	2.5	0.068	0.045	1.085	0.031	1.072	1	0	0.35	0.55	0	0
GRE_E (GREENS energy type)	0.225	0.275	0.0238	0.0018	0.033	2.5	0.068	0.035	1.08	0.031	1.072	1	0	0.35	0.55	0	0
FDL_E (Fresh DIATOMS energy type)	0.27	0.21	0.018	0.66	0.04	3	0.35	0.035	1.08	0.031	1.072	1	0	0.35	0.55	0	0
BLU_N (BLUEGRN nitrogen type)	0.2875	0.125	0.0188	0.0018	0.02	2.5	0.048	0.045	1.085	0.012	1.072	1	0	0.35	0.62	0	0
BLU_P (BLUEGRN phosphorus type)	0.2875	0.15	0.015	0.0018	0.02	2.5	0.048	0.045	1.085	0.012	1.072	1	0	0.35	0.62	0	0
ULS_N (Ulva suspended nitrogen type)	0.248	0.033	0.00667	0	0.001	3.3	0.05	0.125	-25	0.01	1.066	1	0	0.3	0.7	0	2
ULS_E (Ulva suspended energy type)	0.248	0.0594	0.01	0	0.001	3.3	0.06	0.125	-25	0.01	1.066	1	0	0.3	0.7	0	1
ULS_P (Ulva suspended phosphorus type)	0.248	0.0594	0.00333	0	0.001	3.3	0.05	0.125	-25	0.01	1.066	1	0	0.3	0.7	0	3
ULF_N (Ulva attached nitrogen type)	0.0248	0.0594	0.00333	0	0.0001	3.3	0.06	0.075	-25	0.01	1.066	-0.25	0	0.3	0.7	0	-3
ULF_P (Ulva attached phosphorus type)	0.0248	0.033	0.00667	0	0.0001	3.3	0.06	0.075	-25	0.01	1.066	-0.25	0	0.3	0.7	0	-2
ULF_E (Ulva attached energy type)	0.0248	0.0594	0.01	0	0.0001	3.3	0.08	0.075	-25	0.01	1.066	-0.25	0	0.3	0.7	0	-1

Figure 4.16: Coefficients for the BLOOM algae sub model

4.9 Dispersion coefficients

4.9.1 Horizontal dispersion

A homogeneous horizontal dispersion coefficient is set by double clicking *Project/water quality model/input/horizontal dispersion*.

Start Page		Water quality model		Water quality model:Dispersion	
Name	Description	Function type	Default value	Unit	Edit
Dispersion	Horizontal Dispersion	Coverage	1	m2/s	...

Figure 4.17: Horizontal dispersion

For setting a spatially variable horizontal dispersion, you select a “Coverage” in the function type column.

Note: Note that a spatially variable horizontal dispersion is indicated in the project explorer.



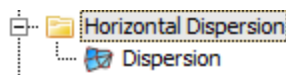


Figure 4.18: Indication in project explorer of horizontal dispersion Dispersion

By clicking in the *Edit* column you activate the Spatial Editor. See the Initial Conditions section for more details.

Additional options are available via the water quality model properties.

Dispersion options	
Horizontal dispersion	1
(Additional) vertical dispersion	1E-07
No dispersion if the flow is zero	False
No dispersion over openbound	True

Figure 4.19: Dispersion options (horizontal)

Horizontal dispersion

This is the same value as discussed above if there is a homogeneous horizontal dispersion. If the horizontal dispersion is a spatial field, this value is no longer accessible. It will be neglected in the simulation.

No dispersion if the flow is zero

This option switches off dispersion when and where the flow is zero. This is a recommended setting. It avoids undesirable transport over temporary dry cells, and it may enhance convergence of iterative numerical solution methods.

No dispersion over open boundaries

We recommend to use this option. This option implies that over open boundaries having an inflow of water, the transport equals the water flow [m^3/s] multiplied with the boundary concentration [g/m^3] which is what we intuitively assume.

4.9.2 Vertical dispersion

The vertical dispersion coefficient is copied from the hydrodynamics model, if information to do so is passed via the hyd-file. Additional options are available via the water quality model properties.

Dispersion options	
Horizontal dispersion	1
(Additional) vertical dispersion	1E-07
No dispersion if the flow is zero	False
No dispersion over openbound	True

Figure 4.20: Dispersion options (vertical)

(Additional) vertical dispersion

The value specified here is applied on top of the values derived from the hyd-file (if applicable).

4.10 Pollution loads

The Getting Started section explains how to manually add pollution loads.

4.10.1 Properties

Pollution loads have the following properties:

- ◇ a name
- ◇ a horizontal position (X,Y)
- ◇ a vertical position (Z), see [section 4.1.1](#)
- ◇ a load type, see [section 4.13](#)
- ◇ a location alias, see [section 4.13](#)

The WAQ GUI does not support loads distributed over the whole water column.

4.10.2 Importing pollution loads

To import pollution loads, right click on *project/water quality model/input/pollution loads/import*. The supported format is a ArcGIS shape file `<*.shp>`¹

The fields read are:

- ◇ Name: any string
- ◇ Load_Type: any string
- ◇ aliases: any string (see [section 4.13](#))
- ◇ X: a real number
- ◇ Y: a real number
- ◇ Z: a real number

4.10.3 Loads corresponding to sources in the hydrodynamics model

Some hydrodynamic models allow sources and sinks in their water balances, which are not explicitly included in the flow field. In the corresponding D-Water Quality model, a segment with a source will have a closed water balance, and the sum of all outflows and inflows might not be in accordance with the volume change. The information about the source is implicitly included.

The WAQ GUI does not automatically create pollution loads to represent these sources. Instead, we suggest that the user imports them as pollution loads, imports a dataset with the flow data (see Section on Boundary Conditions and Loads Data) and adds one or more datasets with the concentration data. If the same data are used which are used to define the sources in the hydrodynamics model, there should not be any problem.

For D-Water Quality models connecting to Delft3D-FLOW, we note that the sources coordinates can be retrieved at the bottom of the `<*_unstructured.hyd>` file (see [Appendix B](#)).

¹To convert a `<*.csv>` file into a `<*.shp>` file in QGIS:

- (a) Layer/add layer/add delimited text layer.
- (b) Browse for the `<*.csv>` file.
- (c) Select the appropriate fields and options.
- (d) Right click on the created layer (left panel), and choose Save as.
- (f) Browse and enter a file name to export as a `<*.shp>` file.

4.11 Observation point

Chapter [D-Water Quality: Getting started](#) explains how to manually add observation points.

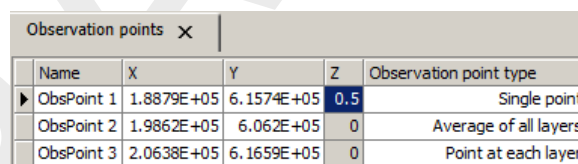
4.11.1 Properties

Observation points have the following properties:

- ◇ a name
- ◇ a horizontal position (X,Y)
- ◇ a vertical position (Z), see [section 4.1.1](#)
- ◇ an observation point type

The observation point type can be:

- ◇ single point: one observation point will be created at the specified value of Z
- ◇ average of all layers: one observation point will be created consisting of all segments in the water column, which implies D-Water Quality will write water column averages
- ◇ point at each layer: multiple observation points will be created, one at each layer for a sigma layer model, one for each active layer for a Z layer model



Name	X	Y	Z	Observation point type
ObsPoint 1	1.8879E+05	6.1574E+05	0.5	Single point
ObsPoint 2	1.9862E+05	6.062E+05	0	Average of all layers
ObsPoint 3	2.0638E+05	6.1659E+05	0	Point at each layer

Figure 4.21: Observation points

4.11.2 Importing observation points

To import observation points right click on *project/water quality model/input/observation points/import*. The supported format is a ArcGIS shape file <*.shp>. ²

The fields read are:

- ◇ Name: any string
- ◇ ObsPt_Type: either
 - SinglePoint
 - Average
 - OneOnEachLayer
- ◇ X: a real number
- ◇ Y: a real number
- ◇ Z: a real number

²To convert a <*.csv> file into a <*.shp> file in QGIS:

- (a) Layer/add layer/add delimited text layer.
- (b) Browse for the <*.csv> file.
- (c) Select the appropriate fields and options.
- (d) Right click on the created layer (left panel), and choose Save as.
- (f) Browse and enter a file name to export as a <*.shp> file.

4.12 Observation areas

There are two ways to define observation areas: manually using the spatial editor, or from an imported shape file.

4.12.1 Define observation areas manually

Double click *project/water quality model/observation areas*.

In the ribbon, choose  **Polygon**. Draw the area and close your polygon by double clicking.

Click  **Set Label** in the ribbon.

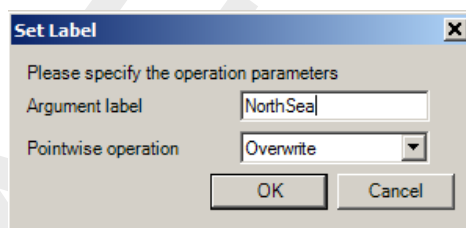


Figure 4.22: Observation areas operation parameters

Type the name of the area, and indicate "Overwrite" (area will be equal to polygon) or "overwrite when missing" (area will be equal to polygon but will not overwrite existing areas).

You may use the spatial operations tools (in the operations panel) to modify the defined area:

- ◇ select the mask corresponding to that area.
- ◇ tick the box to make the mask appear in the map
- ◇ select the polygon, and then use the Edit tools in the ribbon to move/add/remove points of the polygon



Figure 4.23: Edit polygon option in ribbon

- ◇ click *Refresh* in the operations panel to display the changes.

4.12.2 Define observation areas from an imported shape file

Right click on *project/water quality model/observation areas/import*.

Browse and select the appropriate shape file.

4.13 Boundary conditions and loads data

4.13.1 Boundaries and loads

The definition of boundary conditions and loads data proceeds in a very similar way, and will be discussed here. The essential differences between boundary conditions and loads are:

- ◇ boundaries come with the hydrodynamics (hyd-file), loads are added by the user;
- ◇ boundary conditions are specified as g/m^3 , while loads are defined as g/s ;
- ◇ boundary conditions are included in block 5 of the input file, loads data in block 6.

Loads can be specified in two ways:

- ◇ directly as g/s , using the substance names only; or
- ◇ as g/m^3 , using the substance names and an additional variable called FLOW which specifies a discharge in m^3/s .

If the FLOW variable is absent or has a value 0.0, the loads data for individual substances will be interpreted as g/s . In other cases the loads data for individual substances will be interpreted as g/m^3 , and be multiplied with FLOW.

TAKE CARE: if you use the FLOW variable and you want to specify an intermittent load, you need to avoid FLOW values of zero (because this will affect the interpretation of the substance data). Use $\text{FLOW} = 10^{-20}$ instead.

In the remainder of this section we will discuss boundary conditions. The information presented applies to loads data in exactly the same way, with the considerations discussed above.

4.13.2 Functionality of the input processor

The D-Water Quality input processor is very powerful in interpreting input data. The GUI does not duplicate this functionality, but tries to help you to benefit from it in an optimal way.

Things the D-Water Quality input processor can do for you:

- ◇ merge different data tables: if you have input data from different sources, you do not have to merge them yourself;
- ◇ deal with time series with uneven intervals;
- ◇ deal with incomplete data: if your data set lacks some variables, D-Water Quality will assume zeroes or allows you to set a default value;
- ◇ deal with missing values: if your data set has missing values for certain variables at certain times, you do not have to worry about interpolating;
- ◇ convert measured variables to simulated substances (also known as “USEFOR” functionality): DELWAQ offers intricate calculation algorithms that allow you for example to split up a measured value of total nitrogen into the modelled substances PON_1 , NH_4 and NO_3 ;
- ◇ deal with different location names in the input data and your model: you do not have to carry out cumbersome “search and replace” actions.

4.13.3 Working with data sets

The GUI works with data sets. A data set is defined as:

- ◇ a sequence of values for a certain location, a certain variable and a certain time,
- ◇ optionally specifying values for different locations,
- ◇ optionally specifying values for different variables,
- ◇ optionally specifying values for different times,
- ◇ without the need to specify values for all locations and variables at all times,
- ◇ using either BLOCK or LINEAR interpolation,
- ◇ using a single set of USEFOR rules to convert the variables in the data set to modelled substances.

In practice, we recommend using a single data set for data you retrieve from a single source. The only restrictions are that a single set of USEFOR rules should apply to the whole data set, and that either linear or block interpolation is used for the whole dataset. If this is not feasible, it is necessary to split the data set.

The GUI allows you to perform the following actions on your data sets.

Import a dataset

Import a dataset by right clicking *Project/water quality model/input/boundary data /import*.

The file

```
timeBlock,location,substance,value
1990-01-01 00:00:00,SEA BOUNDARY,OXY,7
1990-01-01 00:00:00,SEA BOUNDARY,NH4,0.1
```

will result in:

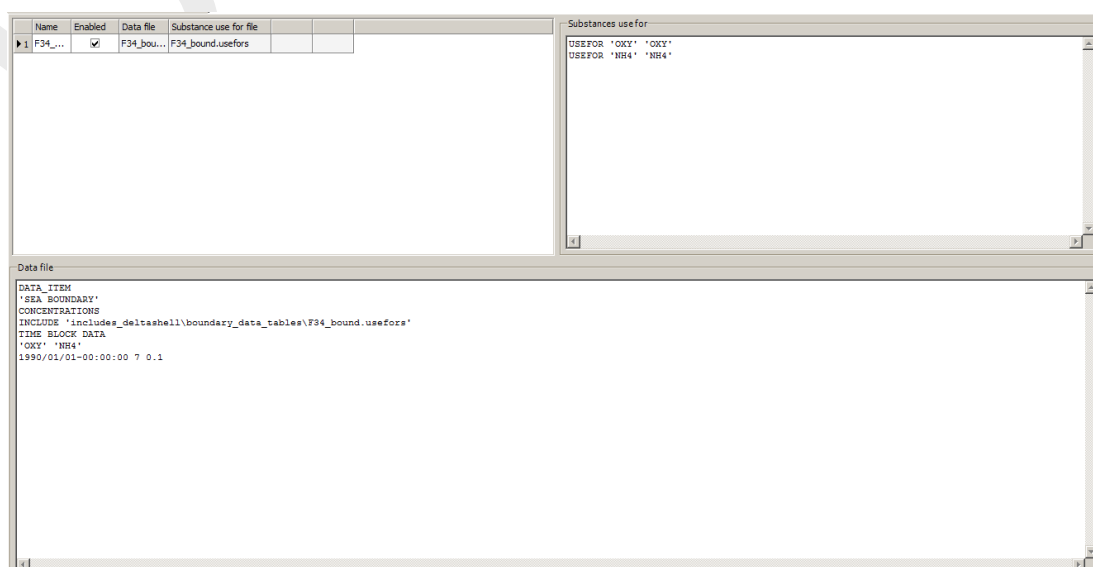


Figure 4.24: Showing import result of a dataset

This window shows the data set list (top left), the imported data set translated to the D-Water Quality keyword based format (bottom) and the substance aliases section (top right).

Name a dataset

Change the name field in the data set list (top left).

Activate and deactivate a dataset

Tick or untick the Enabled field in the data set list (top left).

Delete a dataset

Doubleclick the line number in the data set list (top left) to select the data set. Use right click *delete* to delete the dataset.

Add a set of USEFOR rules to the dataset

After importing a dataset, all data set variables are aliased to themselves, e.g.

```
USEFOR `OXY' `OXY'
```

This will be sufficient if the data set variables are the same as the modelled substances. If that is not the case, you can edit the USEFOR rules manually (top right). Below, we provide further information.

Determine the priority of one dataset relative to the others

If you import more than one dataset, arrows will appear in the data set list (top left) allowing you to change their order. This is only relevant if individual data sets define time series for the same variables and locations. The order of the datasets in the list will determine the order of the data in the D-Water Quality input file. Following the D-Water Quality input processor logic, the data set last read will overrule the earlier data sets (insofar as duplicate information is included).

4.13.4 Supported data set formats

Simple table in csv format

Fields:

- ◇ timeBlock or timeLinear
- ◇ location
- ◇ substance
- ◇ value

Per location, the times have to be sequential.

Example:

```
timeBlock,location,substance,value  
1990-01-01 00:00:00,SEA BOUNDARY,OXY,7  
1990-01-01 00:00:00,SEA BOUNDARY,NH4,0.1
```

The use of `timeBlock` or `timeLinear` columns decides if D-Water Quality will use block or linear interpolation.

4.13.5 Substance aliases (“USEFOR rules”)

Substance aliasing allows you to organize the relations between the variables in the data set and the modelled substances. Below we present some examples. For a full account we refer to the D-Water Quality Description of Input File, section 5.4.2.

Note: ALWAYS USE BLANKS TO SEPARATE THE KEYWORDS, NUMBERS, ARITHMETIC OPERATORS, ETC.



Rename an input variable

```
USEFOR `OXY' `DO'
```

This will rename the input variable ‘DO’ to the modelled substance ‘OXY’.

Scale or split up an input variable

```
USEFOR `NH4' `TotN' * 0.2
```

This will define a value equal to 0.2 times the value of the input variable ‘TotN’ for the modelled substance ‘NH4’.

```
USEFOR `NH4' `TotN' * 0.2
USEFOR `NO3' `TotN' * 0.5
USEFOR `PON1' `TotN' * 0.3
```

This will split up the value of the input variable ‘TotN’ over three modelled substances ‘NH4’, ‘NO3’ and ‘PON1’, according to a fixed 2:5:3 ratio.

Add or subtract input variables

```
USEFOR `NO3' `Nitrates' + `Nitrites'
```

This will assign the sum of the input variables ‘Nitrites’ and ‘Nitrates’ to the modelled substance ‘NO3’.

```
USEFOR `PON1' `KjeldahN' - `Ammonium' MIN 0.0
```

This will assign the difference of the input variables ‘KjeldahN’ and ‘Ammonium’ to the modelled substance ‘PON1’. The MIN keyword followed by a value of 0.0 ascertains that the result of the operation will not become negative.

TAKE CARE: by using the MIN keyword, you may cause mass errors. For example:

```
USEFOR `PON1' `KjeldahN' - `Ammonium' MIN 0.0
USEFOR `NH4' `Ammonium'
```

In this case, the sum of the values obtained for the substances ‘PON1’ and ‘NH4’ can be bigger than the value for the input variable ‘KjeldahN’ (if ‘Ammonium’ > ‘KjeldahN’).

Multiple operations

It is possible to combine the above options, for example:

```
USEFOR `S1' `I1' * 2.  
-- `I2' / 3.  
MIN 0.1
```

Where S1 is a modelled substance and I1 and I2 are input variables. The input processor will use the normal mathematics convention that the '*' and the '/' are evaluated before '-' and '+'. So: if I1 = 3 and I2 = 3, S1 will be $3*2 - 3/3 = 6 - 1 = 5$.

And if I1 = 1 and I2 = 6, S1 would be $1*1 - 6/3 = 1 - 2 = -1$, but the MIN operator will cause S1 to be equal to 0.1.

Add a default value for a modelled substance

```
USEFOR `OXY' 8.0
```

This will give the modelled substance OXY, which is apparently not included in the dataset, a value of 8.0.

4.13.6 Location aliases

Both boundaries and loads can be given "location aliases".

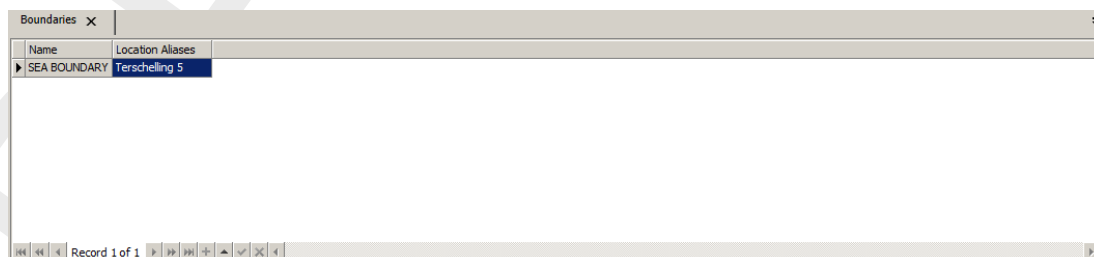


Figure 4.25: Location aliases for boundaries

Values in any of your datasets for the location 'Terschelling 5' will be used as boundary concentrations for the boundary called "SEA BOUNDARY".

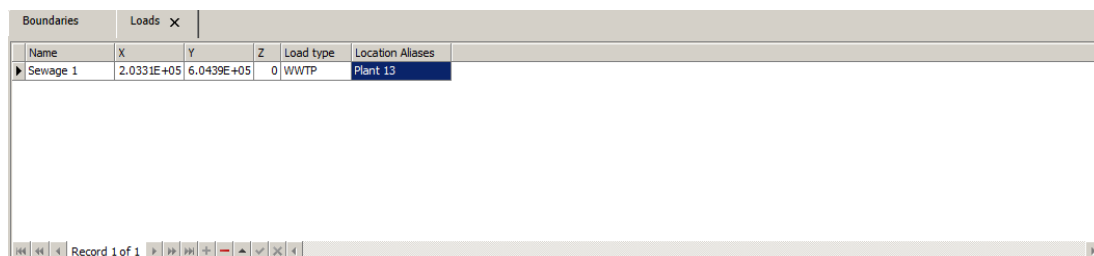


Figure 4.26: Location aliases for load data

Values in any of your datasets for the location 'Plant 13' will be used as load data for the load called 'Sewage 1'.

You can use multiple location aliases, they need to be separated by commas.

4.13.7 Load types; setting defaults

Optionally, you can define a type for the loads. Typically you do this if you want to cluster your loads. Clustering allows you to set default values for the loads from a certain type of sources, which you can overrule for individual loads with specific data.

An example:

Name	X	Y	Z	Load type	Location Aliases
Sewage 1	2.0331E+05	6.0439E+05	0	WWTP	Plant 13
Sewage 2	1.9802E+05	6.0907E+05	0	WWTP	Elm Road

Figure 4.27: Setting default values for Load types

In this case you could use three datasets:

Dataset 1: contains effluent values for all plants (variable 'FLOW')

Dataset 2: contains default concentrations of pollutants in WWTP effluents (location 'WWTP')

Dataset 3: contains actual data for effluent concentrations (location 'Plant 13', 'Elm Road').

By defining them in this order, the default values from Dataset 2 will be used for loads and substances not covered by Dataset 3. However, loads and substances data from Dataset 3 will overrule the defaults in Dataset 2.

The equivalent functionality for boundaries is not yet implemented.

4.14 Mass balances

You access the mass balances output options in the properties panel by a right click on *project/water quality model*. These options are intended to allow you to manage the size of the output files and the amount of detail for your interpretation of the output.

Balance options	
Balance active	False
Balance output unit	Gram
Lump processes	True
Lump boundaries and loads	True
Lump transport	True
Suppress time dependent output	True
Suppress space	True
No balance (monitoring points)	True
No balance (monitoring areas)	True
No balance (model wide)	False

Figure 4.28: Balance options

Balance active

Activates the “extended mass balances” (keyword) BALANCES-SOBK-STYLE. This will result in <*_bal.his> and <*_bal.prn> output files. The former provides mass balances per output period interval, while the latter provides mass balances for the complete output period.

Balance output unit

This refers to the unit used in the <*_bal.his> file. The <*_bal.prn> presents the output in all possible units.

Lump processes

Controls option to have output for all processes together, or for individual processes

Lump boundaries and loads

Controls option to have output for all boundaries and loads together, or for individual boundary and load types

Lump transport

Controls option to have all internal transports lumped, or to have output for all fluxes between individual monitoring points/areas

Suppress time dependent output

Controls the writing of the <*_bal.his> file

Suppress space (dependent output)

Controls the writing of output for individual monitoring points/areas or just their total

No balance (monitoring points)

Controls option to omit monitoring points from the balances

No balance (monitoring areas)

Controls option to omit monitoring areas from the balances

4.15 Run simulation

See the [chapter 3](#) for a description how to run a simulation.

4.15.1 Model validation

For model validation the WAQ GUI has basic functionality. The validation tool can be accessed by a right mouse click on *project/waterquality model/validate*. It will always come up if a simulation does not end correctly.



Figure 4.29: Model validation result

The validation of the details of the input is done by the D-Water Quality input processor, which constitutes the first step of a simulation, see the section on Troubleshooting.

4.15.2 Troubleshooting

After the completion of the simulation, you can inspect messages from the D-Water Quality computational program as items in the project explorer under "Output":

- ◇ List file: <*.lst> from the input processing programme (delwaq1.exe)
- ◇ Process file: <*.lsp> from the input processing programme (delwaq1.exe)
- ◇ Monitoring file: <*.mon> from the simulation programme (delwaq2.exe)

If the simulation has not been successful, the <*.lst>, <*.lsp> and <*.mon> files will help you finding the reason of the problem. Some hints:

- ◇ Read errors are not expected if you use the standard input file. If you chose to edit the input file, this would be the first place to look for possible causes.
- ◇ If there is a read error, you will be able to find which part of the input presents a problem by looking for "Error" in <*.lst>. By going up in the file you can try to identify which information is read correctly and why a problem occurs.
- ◇ Warnings in the <*.lst>. file do not normally occur, and should be checked.
- ◇ Warnings in the <*.lsp> file are more common, but should also be checked:
 - look for the string "can not" to find processes that are requested but can not be switched on due to lack of input data; you may have forgotten to edit a process coefficient which has the missing value -999;
- ◇ Check the bottom of the <*.lsp> file for output items that can not be located: this indicates a problem in the sub file.
- ◇ Check the bottom of the <*.lsp> file for input items that have not been used: this may indicate a problem in the sub file. Please notice that if a process coefficient has been specified as a time series or a spatial field, the constant value may still be in the input file, and will correctly be indicated as not used.
- ◇ A crashing simulation will often produce an error message in the <*.mon>-file. Common messages are:

- the GMRES error indicating a convergence problem in an iterative solver (see Numerical Options).
- messages from specific water quality processes indicating that certain processes coefficients are outside their valid range.
- messages from specific water quality processes indicating that certain processes coefficients have been defined as spatial fields, where this is not allowed.

4.16 Postprocessing

4.16.1 Using Delft3D Flexible Mesh Suite or D-HYDRO Suite.

The postprocessing options offered by the D-Water Quality are discussed in [chapter 3](#).

4.17 Project, model and file management

You manage your projects by using the File menu. A project will be saved in a file *<project name.dsproj>*.

Within each project, you can create one or more models. The first model is created after importing the hyd-file. Any following project can be created by a right mouse click on *project/add/new model* and importing a hyd-file.

Delete a model

Models can be deleted by a right mouse click on *<project/water quality model/delete>*. All data related to these models are in folders placed next to the *<project name.dsproj>* file. For every model there is a folder holding input: *<Water_quality_model>* and a folder holding results: *<Water_quality_model_output>*

Remark:

- ◇ You can delete a project by deleting the dsproj-file and the associated model folders. This should be done with care!



Note: If you include your own files by editing the input file, make sure to store these files OUTSIDE the model folders that the GUI creates.

5 Conceptual description

5.1 Introduction

D-Water Quality solves the equations for transport and physical, (bio)chemical and biological processes. You need to define transport and processes and the model does the rest. However, you should be familiar with the basic concepts in order to understand the functioning of D-Water Quality and to make optimal use of the multiple possibilities of the program.

In this chapter we introduce the mathematical '*advection-diffusion-reaction equation*' that forms the basis of D-Water Quality. As the model makes use of discrete computational elements and discrete time steps, this analytical equation can not be applied directly. Therefore, we will introduce you to the numerical discretisation of D-Water Quality and the underlying principles of how to describe transport and water quality processes.

5.2 Mass balances

D-Water Quality administrates the mass balance of selected state variables, such as dissolved oxygen, nitrate or cadmium. It does so for each computational cell. Mass transported by flowing water from one cell to the next serves as a negative term in the mass balance in the first computational cell and as a positive term in the second computational cell. The method is mass-conserving by definition. By combining computational cells in one, two or three dimensions each water system can be represented and substances can be transported through computational cells and hence through the water system. When we take into account that within a computational cell substances can be converted to other substances, we have to include water quality processes. For example, nitrification converts ammonium (NH_4^+) to nitrate (NO_3^-), resulting in a negative term in the ammonium mass balance of that computational cell and a positive term in the nitrate mass balance. Finally, we can add mass to a computational cell that originates from outside the modelled water system. Waste loads are an example of this, but also mass may also enter the modelled water system across open model boundaries.

To proceed one step in time ($t + \Delta t$), D-Water Quality solves Eq.(5.1) for each computational cell and for each state variable. Eq.(5.1) is a simplified representation of the advection-diffusion-reaction equation which will be discussed in [section 5.4](#).

$$M_i^{t+\Delta t} = M_i^t + \Delta t \times \left(\frac{\Delta M}{\Delta t} \right)_{Tr} + \Delta t \times \left(\frac{\Delta M}{\Delta t} \right)_P + \Delta t \times \left(\frac{\Delta M}{\Delta t} \right)_S \quad (5.1)$$

The mass balance has the following components:

- ◇ the mass at the beginning of a time step: M_i^t
- ◇ the mass at the end of a time step: $M_i^{t+\Delta t}$
- ◇ changes by transport: $\left(\frac{\Delta M}{\Delta t} \right)_{Tr}$
- ◇ changes by physical, (bio)chemical or biological processes: $\left(\frac{\Delta M}{\Delta t} \right)_P$
- ◇ changes by sources (e.g. waste loads, river discharges): $\left(\frac{\Delta M}{\Delta t} \right)_S$

It should be noticed that the basic principles of D-Water Quality are the same whether you have one state variable and only two computational cells, or you have several tens of state variables and thousands of computational cells. The only difference is the number of times that D-Water Quality has to solve Eq.(5.1).

Changes by transport include both advective and dispersive transport, that is the transport by flowing water and the transport as a result of concentration differences respectively. The



flow of water is usually derived from the Delft3D-FLOW or D-Flow FM hydrodynamic models (Deltares, 2024h,a). Dispersion in the vertical direction which is important if the water column is stratified, is derived from the hydrodynamic model as well. Dispersion in the horizontal direction is user input (refer to ??). Dispersion, as defined here, differs from the physical concept of molecular diffusion as it stands for all transport that is not described by the advective transport (there is sub grid-scale transport of water that is not resolved by the hydrodynamic model).

Changes by processes include physical processes such as reaeration and settling, (bio)chemical processes such as adsorption and denitrification and biological processes such as primary production and predation on phytoplankton. Water quality processes convert one substance to another (such as the aforementioned nitrification example). A special type of processes deals with settling in a 3-dimensional situation, as these processes transport particulate matter from one computational cell to the one below. For a detailed description of the water quality processes included in D-Water Quality refer to chapter 6 and the D-Water Quality Technical Reference Manual (Deltares, 2024e).

Changes by sources include the addition of mass by waste loads and the extraction of mass by intakes. Mass entering over the model boundaries can be considered a source as well. The water flowing into or flowing out of the modelled area over the model boundaries is derived from the hydrodynamic model.

5.3 Spatial schematisation

To model the transport of substances, a water system is divided in small boxes (Figure 5.1). The complete ensemble of all the small boxes is called the 'grid' or 'schematisation'. In D-Water Quality each box — from now on called a computational cell — is defined by its volume and its dimensions in one, two or three directions (Δx , Δy , Δz) depending on the nature of the schematisation (1D, 2D or 3D). Note that Δx , Δy and Δz do not have to be equal, so that the computational cell can have any rectangular shape. A computational cell can share surface areas with other computational cells, the atmosphere and the sediment or coast line.

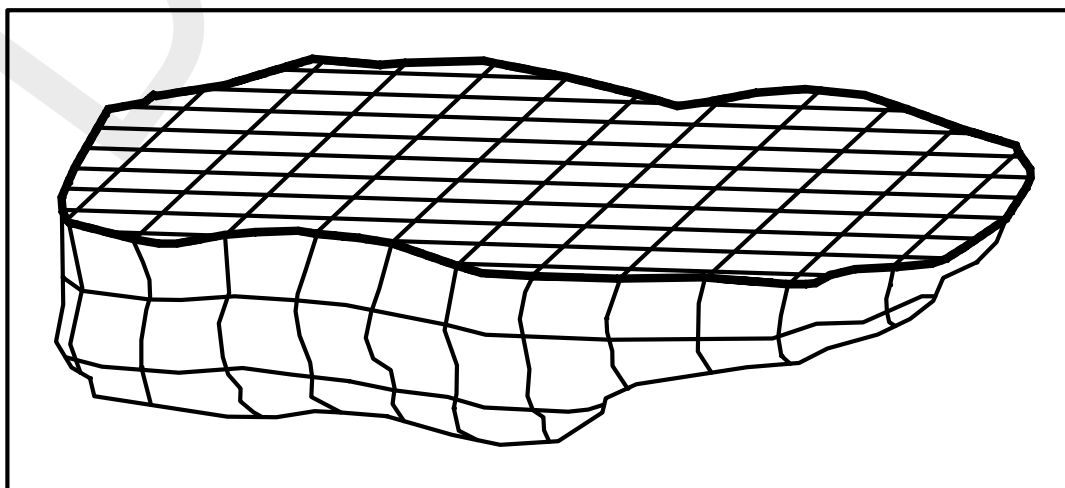


Figure 5.1: Division of a lake into small boxes with a finite volume; a structured three dimensional grid is used

In D-Water Quality each computational cell has a unique number ranging from 1 to N, where N is the total number of computational cells. Also, each surface area that is shared with another computational cell, is identified by a unique number, ranging from 1 to Q, where Q is the total number of shared surface areas. Over this shared surface area mass can be

exchanged between computational cells. Therefore, the shared surface areas are referred to as *exchanges* as well. D-Water Quality defines an exchange by the numbers of the two computational cells that share the surface area.

Recapitulating, for each computational cell we know its:

- ◇ volume
- ◇ dimensions
- ◇ surface area
- ◇ neighbouring computational cells (i.e. exchanges)

Thus, we describe a water system in individual computational cells and through the exchanges we know how the individual computational cells are interconnected. Adding to this the flow of water between the computational cells which is derived from the hydrodynamic model (D-Flow FM, Delft3D-FLOW, ...), and the basis for water quality modelling is there. Substances and water quality processes can be added.

Because D-Water Quality derives flows, volumes and the geometry from the hydrodynamic model, you do not need to define them yourself. An example of a schematisation for D-Water Quality is shown in [Figure 5.2](#).

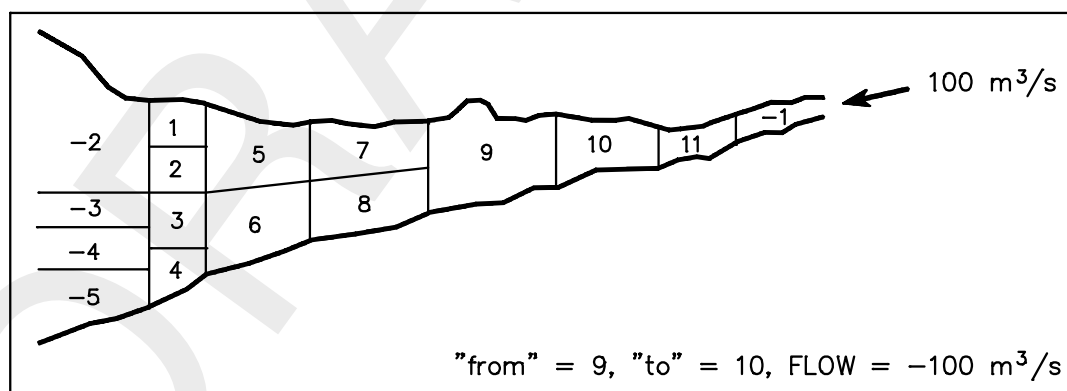


Figure 5.2: Schematisation of an estuary with 11 computational cells and 5 boundary cells indicated with a negative number. The exchange table indicates how the computational cells are connected to each other and what the flow between the computational cells is. The "From-1" and "To+1" columns refer to second order connections which are used in some higher order numerical schemes.

Exchange Number	"From"	"To"	"From - 1"	"To + 1"	"Flow"
1	-1	11	-1	10	100
2	11	10	-1	9	100
3	9	10	8	11	-100
4	9	8	10	6	75
5	9	7	10	5	25
6	8	7	0	0	5
7	7	5	9	2	30
8	8	6	9	3	70
9	5	6	0	0	0
10	5	2	7	-2	25
11	5	1	7	-2	5
12	1	2	0	3	0
13	2	3	1	4	0
14	3	4	2	0	5
15	6	3	8	-3	60
16	6	4	8	-5	10
17	3	-3	6	-3	50
18	3	-4	6	-4	5
19	4	-4	6	-4	5
20	4	-5	6	-5	10
21	1	-2	5	-2	5
22	2	-2	5	-2	25



Note: that you have to define 11 volumes but 22 flows to define the transport of water through this estuary completely.

5.4 Advection-diffusion equation

A water quality model is in fact not more than a *mass balance* for the pollutants or state variables necessary to describe the problem at hand. D-Water Quality makes this mass balance for you, for so-called *segments* (i.e. small water volumes):

$$\frac{\partial M}{\partial t} = \text{advection} + \text{dispersion} + \text{source} \quad (5.2)$$

The source term consists for example of direct inputs and/or mortality (for bacteria), decay (for bod), sedimentation (for solid particles), etc.

5.4.1 Advective transport

The advective transport across an exchange can be given as:

$$T_{x_0}^A = v_{x_0} \times A \times C_{x_0}$$

with:

$T_{x_0}^A$	advective transport at $x = x_0$ [g/s]
v_{x_0}	velocity at $x = x_0$ [m/s]
A	surface area at $x = x_0$ [m ²]
C_{x_0}	concentration at $x = x_0$ [g/m ³]

We assume that velocities and concentrations are an average representative value for the whole surface. The smaller the cross section, the better this assumption.

5.4.2 Dispersive transport

The dispersive transport across an exchange is assumed to be proportional to the concentration gradient and to the surface area:

$$T_{x_0}^D = -D_{x_0} \times A \times \left. \frac{\partial C}{\partial x} \right|_{x=x_0}$$

with:

$T_{x_0}^D$	dispersive transport at $x = x_0$ [g/s]
D_{x_0}	dispersion coefficient at $x = x_0$ [m ² /s]
A	surface area at $x = x_0$ [m ²]
$\left. \frac{\partial C}{\partial x} \right _{x=x_0}$	concentration gradient at $x = x_0$ [g/m ⁴]

Dispersion is done according to Fick's diffusion law. The proportionality constant D is called the dispersion (or diffusion) coefficient. The minus sign originates from the fact that dispersion causes net transport from higher to lower concentrations, so in the opposite direction of the concentration gradient.

The concentration gradient is the difference of concentrations per unit length, over a very small distance across the cross section:

$$\left. \frac{\partial C}{\partial x} \right|_x = \lim_{\Delta x \downarrow 0} \frac{C_{x+\frac{1}{2}\Delta x} - C_{x-\frac{1}{2}\Delta x}}{\Delta x}$$

A numerical expression for this term will be given later on. Dispersion coefficients should be calibrated or be obtained from calculations with turbulence models.

5.4.3 Transport from sources

The transport of pollutants from sources is given by the following expression, regardless of the numerical method applied:

$$T_{src} = Q_{src} \times C_{src} \quad Q_{src} > 0 \quad (5.3)$$

If the discharge flow Q_{src} is negative (*withdrawal*), the model uses the following expression:

$$T_{src} = Q_{src} \times C_i \quad Q_{src} < 0 \quad (5.4)$$

where C_i represents the concentration in the receiving Water Quality-segment. Thus, the model withdraws water with the ambient concentrations. The source concentrations supplied by the user are therefore neglected if the discharge is negative (*withdrawal*).

The model mixes the pollutants from the discharge over the receiving Water Quality-segment. So, some erroneous upstream transport of pollutants can not be avoided. If this is not acceptable, the only practical solution is to add more calculation points.

Remarks:

- ◇ There is *no dispersive transport* related to a discharge.
- ◇ If a (lateral) discharge is situated exactly on a calculation point (obligatory in SOBEK-Rural/Urban): SOBEK-River divides the discharge over the grid cells upstream and downstream of the calculation point;
- ◇ SOBEK-Rural/Urban puts the discharge in the reach-segment downstream of the calculation point, where the definition of "downstream" is evaluated based on the local and actual direction of flow.

5.4.4 Mass transport by advection and dispersion

If the advective and dispersive terms are added and the terms at a second surface are included (left and right side of a volume), the one dimensional equation results:

$$M_i^{t+\Delta t} = M_i^t + \Delta t \times A \times \left(v_{x_0} C_{x_0} - v_{x_0+\Delta x} C_{x_0+\Delta x} - D_{x_0} \left. \frac{\partial C}{\partial x} \right|_{x_0} + D_{x_0+\Delta x} \left. \frac{\partial C}{\partial x} \right|_{x_0+\Delta x} \right)$$

with:

M_i^t	mass in volume i at time t [g]
Δt	time step [s]
$\left. \frac{\partial C}{\partial x} \right _{x_0}$	concentration gradient at $x = x_0$ [g/m]
A	surface area [m ²]
v_{x_0}	velocity at $x = x_0$ [m/s]
C_{x_0}	concentration at $x = x_0$ [g/m ³]

Instead of this equation, D-Water Quality uses the following *equivalent* equation:

$$M_i^{t+\Delta t} = M_i^t + \Delta t \times \left(Q_{x_0} C_{x_0} - Q_{x_0+\Delta x} C_{x_0+\Delta x} - D_{x_0} A_{x_0} \left. \frac{\partial C}{\partial x} \right|_{x_0} + D_{x_0+\Delta x} A_{x_0+\Delta x} \left. \frac{\partial C}{\partial x} \right|_{x_0+\Delta x} \right)$$

with:

M_i^t	mass in volume i at time t [g]
Δt	time step [s]
$\left. \frac{\partial C}{\partial x} \right _{x_0}$	concentration gradient at $x = x_0$ [g/m]
A_{x_0}	surface area at $x = x_0$ [m ²]
Q_{x_0}	flow at $x = x_0$ [m ³ /s]
C_{x_0}	concentration at $x = x_0$ [g/m ³]

If the previous equation is divided by the volume $V = \Delta x \Delta y \Delta z^1$ and the time span Δt , then the following equation results in one dimension.

$$\frac{C_i^{t+\Delta t} - C_i^t}{\Delta t} = - \frac{v_{x_0+\Delta x} C_{x_0+\Delta x} - v_{x_0} C_{x_0}}{\Delta x} + \frac{D_{x_0+\Delta x} \left. \frac{\partial C}{\partial x} \right|_{x_0+\Delta x} - D_{x_0} \left. \frac{\partial C}{\partial x} \right|_{x_0}}{\Delta x} +$$

Taking the asymptotic limit $\Delta t \rightarrow 0$ and $\Delta x \rightarrow 0$, the advection-diffusion equation for one dimension results:

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(vC) - \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) = 0$$

¹ Hereto it is required that all segments have an equal volume.

Thus, the finite volume method for transport is a computational method to solve the advection-diffusion equation. The accuracy of the method will be related to the size of Δx , $A (= \Delta y \times \Delta z)$ and Δt .

By adding terms for transport in the y - and z -direction a 3-dimensional model is obtained. Taking the asymptotic limit again, will lead to a 3-dimensional advection-diffusion equation:

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} - D_x \frac{\partial^2 C}{\partial x^2} + v_y \frac{\partial C}{\partial y} - D_y \frac{\partial^2 C}{\partial y^2} + v_z \frac{\partial C}{\partial z} - D_z \frac{\partial^2 C}{\partial z^2} = 0 \quad (5.5)$$

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} - D_x \frac{\partial^2 C}{\partial x^2} + v_y \frac{\partial C}{\partial y} - D_y \frac{\partial^2 C}{\partial y^2} + v_z \frac{\partial C}{\partial z} - D_z \frac{\partial^2 C}{\partial z^2} = S + f_R(C, t) \quad (5.6)$$

with dispersion coefficients taken for every direction. If functions S and f are added as shown in the equation above, the so-called advection-diffusion-reaction equation emerges. The additional terms are so-called source terms. They stand for:

- 1 Discharges or 'waste loads' (S): these source terms are additional inflows of water or mass that were not present in the hydrodynamic module (D-Flow FM, Delft3D-FLOW, SOBEK). They may be present in the continuity equation, but this is not strictly required. As many source terms as required may be added by you. They are usually used for small rivers, discharges of industries, sewage treatment plants, small waste load outfalls, etc.
- 2 Reaction terms or 'processes' (f_R).

Processes can be split into physical processes and other processes. Examples of physical processes are:

- ◇ settling of suspended particulate matter
- ◇ water movement not affecting substances, like evaporation
- ◇ volatilisation of the substance itself at the water surface.

Examples of other processes are:

- ◇ biochemical conversions like ammonia and oxygen forming nitrite
- ◇ growth of algae (primary production)
- ◇ predation by other animals
- ◇ chemical reactions.

Only processes that can be written in the form of a partial differential equation are considered

$$\left(\frac{\partial \bar{C}_1}{\partial t} \right)_R = f_R(\bar{C}_1, \bar{C}_2, \dots, \bar{C}_N, t)$$

with:

\bar{C}_i	concentration at a given location for substance 'i' (here for N substances)
f_R	any functional prescription
t	time

The function describes a relation between the concentration variation at a certain location (x, y, z) and all other concentrations at exactly the same location at that time. Although this is a very general formulation, some types of processes do not fit. Among them is, as most important, the equilibrium kinetics of chemistry. Only relatively slow chemical processes can be described with this equation.

5.5 Boundary conditions

5.5.1 Closed boundaries

Closed boundaries are those boundaries that have zero flow and dispersion for all time steps. No transport is associated with these exchange surfaces. Sometimes exchanges are defined anyway for these boundaries (e.g. for structured grids) in order to keep the grid layout completely structured. In such cases the grid has some permanently dry cells. For closed boundaries no concentrations are required as input.

5.5.2 Open boundaries

Open boundaries are required for solution of the advection-diffusion equation. Without specification of the open boundaries the model does not know what to do at its borders. Concentrations of all substances and dispersion coefficients must be specified at all open boundaries for all time-steps. Flows are automatically taken from D-Flow FM, Delft3D-FLOW or SOBEK. As a consequence of the mathematics behind the Water Quality model, *downstream boundaries* do have an effect on the solution of the Water Quality model:

- ◇ If the advection term is computed by a "*central method*", the concentration at the interface between the last model segment and the downstream boundary is computed as the *average* between the concentration in the last segment and the downstream boundary concentration. Therefore, the downstream boundary concentration affects the advective transport in this case.
- ◇ For the computation of the dispersive term, the concentration gradient at the interface between the last model segment and the downstream boundary is computed as the *difference* between the concentration in the last segment and the downstream boundary concentration divided by the distance between the two. Therefore, the downstream boundary concentration affects the dispersive transport.

D-Water Quality offers the possibility to avoid this effect of downstream boundary concentrations on the solution. You can optionally (1) use an *upwind* advection scheme locally at the model boundaries, and (2) suppress the dispersive transport locally at the model boundaries.

Remark:

- ◇ In [Figure 5.2](#) boundaries are segments with negative numbers. These boundary segments can be considered either as:
 - ◇ inactive computational elements
 - ◇ elements with one cross section but without any volume of water

5.5.3 Time lags and return time

If water crosses a boundary, it may be assumed that the concentration immediately outside of the model area is influenced by the previous outflows. If the flow changes sign and inflow takes place again (as in tidal estuaries), it may be assumed that part of the water flowed out previously, enters again. As inflow proceeds, the boundary conditions as specified by you, may become more and more effective. D-Water Quality enables you to use a cosine shaped function from the last outflow concentration to the specified boundary condition, according to [Figure 5.3](#). This so-called Thatcher-Harleman time lag uses the inner concentration if outflow takes place and starts with the latest outflow concentration to reach the specified boundary concentration within the user specified time lag.

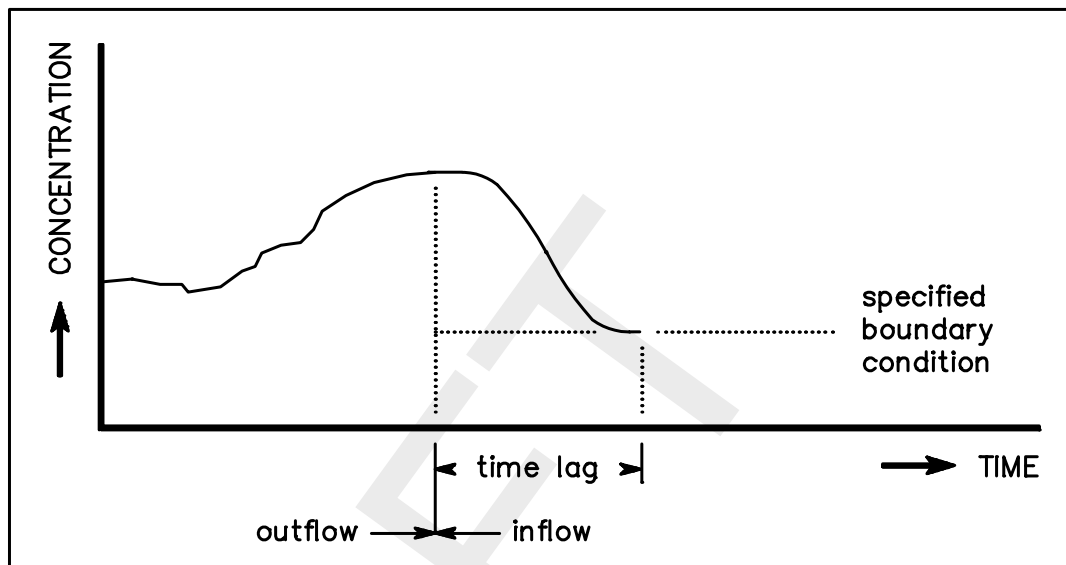


Figure 5.3: Thatcher-Harleman boundary time lag

In mathematical form it is given by:

$$C(t_0 + t) = C(t_0) \left(0.5 + 0.5 \cos \left(\frac{\pi t}{2T} \right) \right) + C_B(t) \left(0.5 - 0.5 \cos \left(\frac{\pi t}{2T} \right) \right) \quad (5.7)$$

with $t_0 < t - t_0 < t_0 + T$, and:

t_0	time that outflow changes to inflow
t	time after t_0
C	simulated boundary concentration
C_B	user-specified boundary concentration (may be time-dependent as well)
T	Thatcher-Harleman time lag

The Thatcher-Harleman time lag T must be specified accurately if the model domain is small with respect to the boundaries. In such cases, the boundary conditions have a large impact on the simulation results. For estuaries it is typically in the order of one to six hours and for polder systems typical values are in the order of five days. For most application the model boundaries will be far from a region of interest (a beach, an ecological site, a dumping site, etc.) and the use of constant boundary conditions will then be sufficient.

DRAFT

6 Principles of water quality modelling

6.1 Introduction

Water quality deals with the composition of water. In its most limited definition, only the chemical composition of a water system is included. However, in D-Water Quality we include biological components up to the level of primary producers and some secondary producers as well as the composition of the sediment in water quality modelling.

In this section we will give a basic outline of water quality in general and a more detailed outline of how water quality processes are implemented in D-Water Quality. The theory of water quality will not be discussed in detail here as we expect the basic knowledge to be present. However, we discuss the principles of water quality as needed to link the text book theory to the D-Water Quality model.

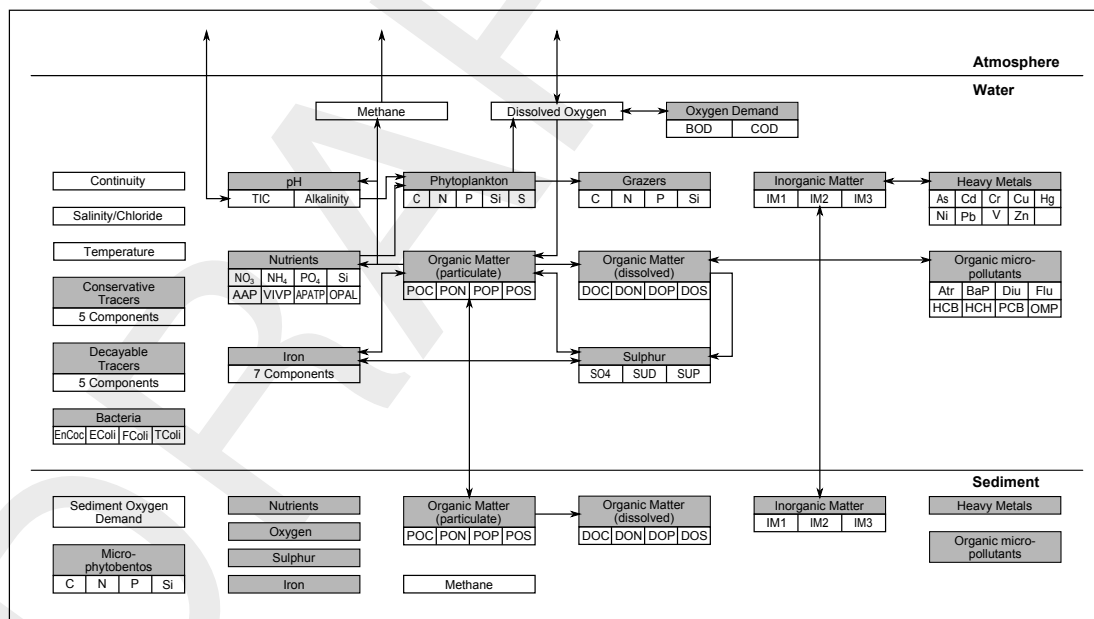


Figure 6.1: General overview of substances included in D-Water Quality. Substances are organised in functional groups indicated by a grey header, except for some substances that form a group of their own. Major links between substances are indicated by arrows; note that many links are omitted.

In D-Water Quality the constituents of a water system are divided in functional groups (Figure 6.1). A functional group includes one or more substances that display similar physical and/or (bio)chemical behaviour in a water system. For example, the nutrients nitrate, ammonium, phosphate and silicon are a functional group as they are required for primary production. Functional groups can interact with each other directly, as in the previous example, or indirectly as inorganic suspended matter influences the light availability for primary production.

In the remainder of this chapter the functional groups are described separately. To get a complete description of the water system you intend to simulate, you will have to combine the separate descriptions of the functional groups. Within the functional group descriptions links to other functional groups are indicated.

6.2 Salinity, chloride, tracers and continuity

Salinity, chloride and conservative tracers are special substances in D-Water Quality as they are not subject to water quality processes. They are only subject to transport. As insight

in transport is usually essential, these substances are nevertheless useful to water quality modellers. Not subject to water quality processes themselves, these substances allow you to distinguish between the effect of transport and processes for other substances, as they can isolate the effect of transport. Obviously, salinity and chloride indicate the fate of fresh river water mixing with sea water.

Conservative tracers (conservative meaning 'not subject to decay') have a wider range of application as they can be assigned at choice to sources of water. You might want to use conservative tracers to indicate where the water entering over the model boundaries is going to, or to determine the fraction of the water originating from a certain source. D-Water Quality allows you to specify up to five conservative tracers.

A special type of conservative tracer is called 'Continuity'. It has no physical or chemical meaning. Instead it is used to establish the numerical correctness and stability of the simulation. By assigning a concentration of 1 g/m³ to all water sources (initial condition, boundary condition and discharges) the Continuity concentration should remain 1 g/m³ during the whole simulation, as there are no processes that dilute or concentrate it and all water has a concentration of 1 g/m³. If the concentration during the simulation significantly deviates from 1 g/m³, you have either overlooked a source of water or the simulation is numerically unstable. You should never proceed with including more substances in the water quality simulation if the latter happens. If for example the Continuity concentration is equal to 1.1 g/m³, the deviation is +10 %. If you included for example nitrate in the simulation, the nitrate concentration would have been overestimated by 10 % as well.

Next to conservative tracers D-Water Quality has five decayable tracers as well. Decayable tracers are subject to first order decay ($C(t) = C_0 \times e^{-k \times t}$). Decayable tracers can represent radioactive elements, when the decay rate k is proportional to the half life ($k = \frac{\ln 2}{t_{1/2}}$). Ignoring the complex chemical reactions and assuming first order decay, decayable tracers have been used to simulate the break-down of disinfectants such as chlorine in the natural environment.

In combination with conservative tracers decayable tracers can be used to establish the 'age' of water from a specific source. The decaying tracer serves as a timer after it is released simultaneously with the conservative tracer.

6.3 Water temperature and temperature dependency of rates

The water temperature determines the rate at which water quality processes take place. As such, it is important that the water temperature is correct in the simulation. The temperature dependency of reaction rates has a uniform exponential [Equation \(6.1\)](#) that is applied in many of the processes included in D-Water Quality:

$$k = k^{20} \times k_T^{(T-20)} \quad (6.1)$$

with:

k	rate constant at temperature T [d ⁻¹]
k^{20}	rate constant at reference temperature 20 °C [d ⁻¹]
k_T	temperature coefficient [-]
T	ambient water temperature [°C]

The temperature coefficient k_T usually ranges between 1.01 and 1.10. With a value of 1.04 the reaction rate at 10 °C is 68 % of the rate at 20 °C. A value of 1.07 results in a doubling or halving of a reaction rate every 10 degrees increase or decrease respectively.

D-Water Quality allows you to calculate the ambient water temperature as a function of the ambient air temperature. The heat gain from or loss to the atmosphere takes into account the wind speed. You can choose to simulate the absolute temperature or the surplus temperature. The latter is useful when simulating the discharge of cooling water used for example by power plants.

The more elaborate temperature modelling through solar radiation, cloudiness, (back-)scattering, evaporation, etc. is implemented in D-Flow FM or Delft3D-FLOW (Deltares, 2024a,h).

Note: that if the water temperature was included in the D-Flow FM, Delft3D-FLOW simulation, it is an option to include this in D-Water Quality as a segment (forcing) function.



6.4 Coliform bacteria

6.4.1 Concepts

Coliform bacteria can be modelled as stand-alone substances.

Coliform bacteria originate from human and animal faeces and are often used as indicator for the presence of disease vectors.

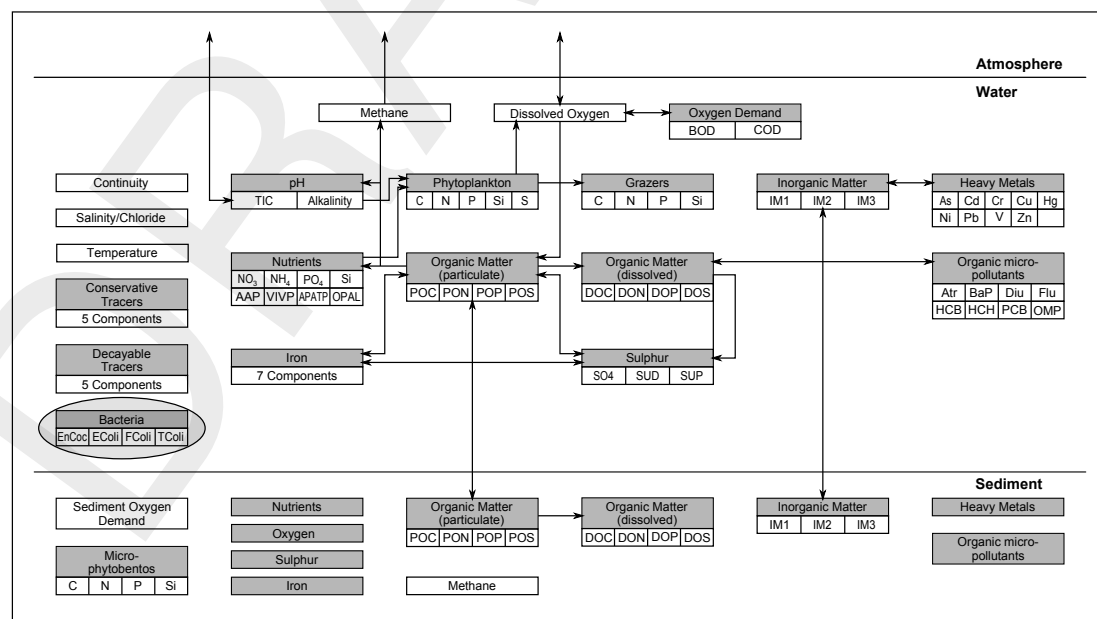


Figure 6.2: Overview of substances. Coliform bacteria

As soon as coliform bacteria are discharged into surface water, they start to die since the conditions that these bacteria meet are essentially hostile to them. The mortality of coliform bacteria is enhanced by temperature, salinity and solar radiation. The lethal effect of light is associated with short wavelengths.

6.4.2 Modelling framework

The substances that can be modelled in D-Water Quality in relation to bacterial pollution are:

Name of D-Water Quality substance	Description	Unit
TCOLI	Total coliforms	MPN/m ³
FCOLI	Faecal coliforms	MPN/m ³
ECOLI	Escherichia Coli	MPN/m ³
ENCOC	Enterococci	MPN/m ³



Note: that the unit (MPN/m³, MPN = Most Probable Number) deviates from the unit that is usually reported for concentrations of coliform bacteria: MPN/100 ml. The conversion factor between the units is $1 \text{ MPN/m}^3 = 1 \times 10^{-4} \text{ MPN/100 ml}$.

It is assumed that:

- 1 Coliform bacteria are present in the water column only. They do not accumulate in or resuspend from sediment.
- 2 Coliform bacteria do not grow in the water column, although in reality some growth immediately after discharge might occur.
- 3 Mortality of coliform bacteria is included as a temperature dependent process, formulated according to first-order kinetics.
- 4 The mortality rate is enhanced by salinity and UV-radiation in an additive way.
- 5 The mortality formulation is identical for each of the three coliform substances (ECOLI, FCOLI, TCOLI, ENCOC). You can define species specific coefficients.

The general mass balance equation for coliform bacteria reads:

$$\frac{\Delta C}{\Delta t} = \text{loads} + \text{transport} - \text{mortality}$$

with:

$$\begin{aligned} C &= \text{concentration of coliform bacteria cells [MPN/m}^3\text{]} \\ t &= \text{time [day]} \end{aligned}$$

6.4.3 Process equation

Available formulations for the *mortality* of coliforms are mainly empirical. The formulations as reported by Mancini (1978) are implemented in D-Water Quality. The basic formulations read:

$$\begin{aligned} Rmrt &= kmrt \times Cx \\ kmrt &= (kmb + kmcl) \times ktmrt^{(T-20)} + kmrd \\ kmcl &= kcl \times Ccl \\ kmrd &= krd \times f(I) \end{aligned}$$

with:

$$\begin{aligned} Cx &= \text{concentration of coliform bacteria species [MPN m}^{-3}\text{]} \\ I &= \text{daily solar UV-radiation at the water surface [W m}^{-2}\text{]} \\ kcl &= \text{chloride related mortality constant [m}^3 \text{g}^{-1} \text{d}^{-1}\text{]} \\ kmb &= \text{basic mortality rate [d}^{-1}\text{]} \end{aligned}$$

$kmcl$	chloride dependent mortality rate [d^{-1}]
$kmrd$	radiation dependent mortality rate [d^{-1}]
$kmrt$	first order mortality rate [d^{-1}]
krd	radiation related mortality constant [$m^2 W^{-1} d^{-1}$]
$ktmrt$	temperature coefficient of the mortality rate [-]
$Rmrt$	mortality rate of coliform bacteria [$MPNm^{-3} d^{-1}$]
T	temperature [$^{\circ}C$]
Ccl	chloride concentration [$g m^{-3}$]

The daily average solar UV-radiation is derived from the total daily radiation of visible light. Moreover, the model takes into account that no significant mortality may occur at low temperatures.

6.5 Dissolved oxygen and BOD

6.5.1 Concepts

The fate of dissolved oxygen is closely linked to the fate of organic matter through:



The equation above is the (simplified) photosynthesis reaction in which organic matter (CH_2O) and dissolved oxygen are formed. For each gram C incorporated into organic matter, 2.67 grams of O_2 are formed which is derived from the ratio of the molar masses $32 g O_2 / 12 gC$. The reverse reaction in which carbon dioxide and water are formed, is the mineralization or degradation reaction of organic matter. This reaction is microbially mediated. The organic matter can be autochthonous to the water system when it is produced locally by primary producers, but can be allochthonous as well when it originates from waste loads such as the sewerage system. The degradability of organic matter usually decreases as organic matter ages.

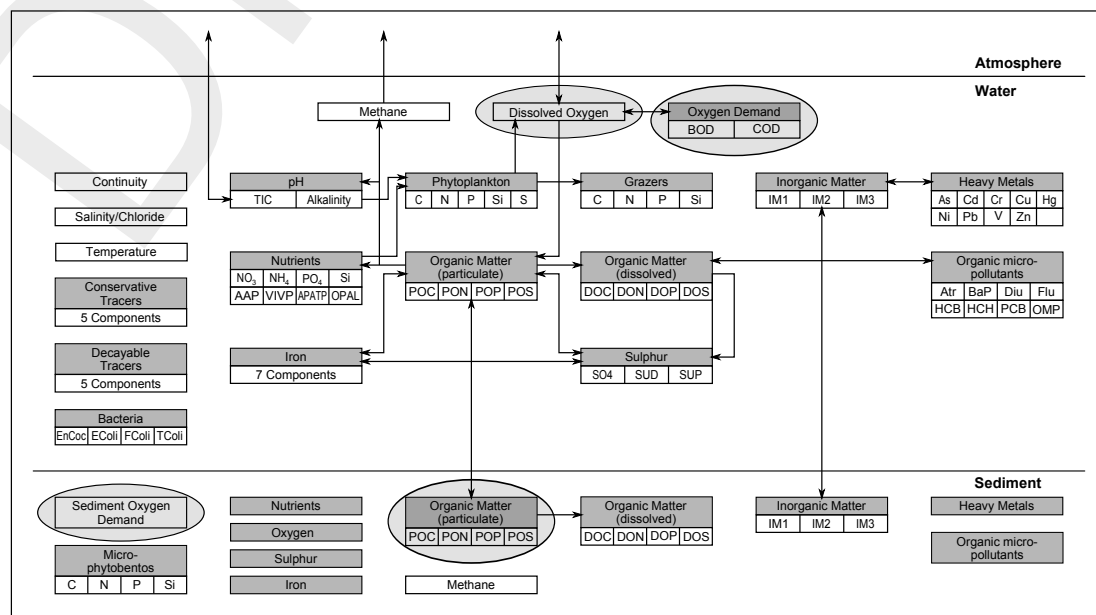


Figure 6.3: Overview of substances. Dissolved oxygen and BOD

In 1925 Streeter and Phelps (Streeter and Phelps, 1925) calculated the so-called dissolved oxygen sag that occurs downstream an organic matter discharge into a river. While the river water flows downstream dissolved oxygen is consumed as organic matter is oxidised. Replenishment from the atmosphere (reaeration) can not match the dissolved oxygen consumption,

until the organic matter amount has been sufficiently reduced. Then the dissolved oxygen concentration will start to rise again as reaeration becomes larger than the oxygen consumption. The point where the lowest dissolved oxygen concentration occurs is called the dissolved oxygen sag.

The Streeter-Phelps approach demonstrates that reaeration is an important source of dissolved oxygen in the water column. Whether or not reaeration will take place depends on the deviation of the actual dissolved oxygen concentration from the saturation concentration at the ambient temperature and salinity. If the actual dissolved oxygen concentration is lower than the saturation concentration, the water is undersaturated and oxygen will enter the water column from the atmosphere. If the actual dissolved oxygen concentration is higher than the saturation concentration, the water is oversaturated and oxygen will escape from the water column to the atmosphere. If the water column is stratified, the hypolimnion is not in contact with the atmosphere as a result of which it can not be replenished and oxygen depletion can occur. Decreased dissolved oxygen concentrations are seen as the major water quality problem arising from stratification.

Finally, dissolved oxygen can be involved in numerous chemical and micro-biological oxidation reactions. The most important reactions are the oxidation of ammonium to nitrate, iron(II) to iron(III), sulphides to sulphate and methane to carbon dioxide and water. Of these reactions only the oxidation of ammonium to nitrate is included in D-Water Quality.

Organic matter in natural waters includes a variety of organic compounds usually present in minute concentrations many of which elude direct isolation and identification. Therefore, collective parameters such as chemical oxygen demand (COD), biochemical oxygen demand (BOD), total organic carbon (TOC), particulate organic carbon (POC) or dissolved organic carbon (DOC) are often used to estimate the quantity of organic matter.

COD is measured using a strong chemical oxidising agent (the Cr-method uses potassium dichromate; the Mn-method uses potassium permanganate). Although it intends to include all oxidisable material, the efficiency of the Cr-method is approximately 90% whereas the Mn-method only yields around 50% of the oxidisable carbon. Ammoniacal and Kjeldahl nitrogen are included in the COD measurement as well as sulphides, methane and other oxidisable material.

BOD consists of carbonaceous and nitrogenous oxygen demand. A much used parameter is BOD₅ (in g O₂/m³) which represents the amount of oxygen that is consumed when a sample is stored for 5 days in a dark environment at 20 °C. As nitrogenous bacteria show a time lag in their growth after incubation, during these 5 days only the carbonaceous oxygen demand is measured.

Discharges of wastes (municipal or industrial) and sewer overflows are principal inputs of oxygen demanding wastes. These discharges cause a chemical oxygen demand (COD), a carbonaceous bio-chemical oxygen demand (CBOD) and a nitrogenous biochemical oxygen demand (NBOD). CBOD represents the oxygen demanding equivalent of the complex carbonaceous material present in waste; NBOD represents the oxygen demanding equivalent of reduced nitrogen species (ammonium or organic nitrogen). Typical values for different waters are presented in.

Table 6.1: Typical values for oxygen demanding waste waters (values in g O₂/m³, data from Thomann and Mueller (1987))

Source	CBOD5	CBODu	NBODu	COD
Municipal waste (untreated)	100–400	220 (120–580)	220	-
Combined sewer overflow (untreated)	170 (40–500)	220	-	-
Separate urban runoff (untreated)	19 (2–80)	-	-	-
Background natural water (excluding algae and detritus)	0	-	-	2–3
Background of natural water (including algae and detritus)	2–3	-	-	10

6.5.2 Modelling framework

The substances that can be modelled in D-Water Quality in relation to dissolved oxygen and dead organic matter (BOD/COD) are:

Name of D-Water Quality substance	Description	Unit
OXY	Dissolved oxygen	g O ₂ /m ³
CBOD5	Carbonaceous Biological Oxygen Demand after 5 days	g O ₂ /m ³
CBODu	Ultimate Carbonaceous Biological Oxygen Demand	g O ₂ /m ³
NBOD5	Nitrogenous Biological Oxygen Demand after 5 days	g O ₂ /m ³
NBODu	Ultimate Nitrogenous Biological Oxygen Demand	g O ₂ /m ³
COD	Chemical Oxygen Demand	g O ₂ /m ³
SOD	Sediment Oxygen Demand	g O ₂

The mass balances for dissolved oxygen, CBOD5 and SOD are given in Equations 6.3, 6.4 and 6.5 respectively. The mass balance for CBOD5 is the same as the mass balances for CBODu, NBOD5, NBODu and COD.

$$\frac{\Delta O_2}{\Delta t} = \text{loads} + \text{transport} + \text{reaeration} + \text{net primary production} \quad (6.3)$$

$$- \text{mineralization} - \text{nitrification} + \text{denitrification}$$

$$\frac{\Delta CBOD5}{\Delta t} = \text{loads} + \text{transport} - \text{settling} - \text{mineralization} \quad (6.4)$$

$$\frac{\Delta SOD}{\Delta t} = \text{loads} + \text{settling} - \text{mineralization} \quad (6.5)$$

In D-Water Quality mineralization of organic matter can be modelled in three ways depending

on the origin of the organic material:

- 1 Organic matter originating from waste water [$\text{g O}_2/\text{m}^3$]
- 2 Detritus organic carbon originating from natural sources such as dead phytoplankton [$\text{g C}/\text{m}^3$]
- 3 The combination of both.

In this section we will only discuss the first option. It can be considered as the representation of the Streeter-Phelps modelling. The second option will be discussed in [section 6.7](#). D-Water Quality allows you to choose both the BOD and the detritus carbon fraction of organic matter (the third option). It is the users responsibility to make sure that no double counting takes place: each carbon atom should belong to one fraction only, either BOD or detritus, and never to both. If this were the case, the oxygen demand would be doubled as both the mineralization of BOD and the mineralization of detritus will consume dissolved oxygen.

Particulate fractions can settle to the sediment¹. The degradation of organic matter continues there². In D-Water Quality all BOD fractions (CBOD5, CBODu, NBOD5, NBODu, COD) are converted to the Sediment Oxygen Demand (SOD) pool when they settle. Mineralization of SOD directly consumes dissolved oxygen in the water column.

Brief description and relevant notes of processes:

Process	Substances	Comments
Reaeration	OXY	<ul style="list-style-type: none"> ◇ The reaeration flux across the air-water interface, which can be positive or negative, is proportional to a reaeration rate constant and the difference between the actual and saturation DO concentrations in water. ◇ The reaeration rate constant can be a function of stream velocity, wind speed and temperature (10 alternative formulations). ◇ The saturation oxygen concentration is a function of water temperature and salinity (2 alternative formulations).
Primary production	OXY (Phytoplankton) (Nutrients)	<ul style="list-style-type: none"> ◇ The production of dissolved oxygen is proportional to the net primary production flux according to $2.67 \text{ gO}_2/\text{gC}$.
continued on next page		

¹For a description of the settling process refer to [section 6.6](#)

²For a detailed description of sediment processes refer to [section 6.11](#)

continued from previous page

Process	Substances	Comments
Nitrification ³	OXY (NH4) (NO3)	$NH_4^+ + 2O_2 \rightarrow NO_3^- + 2H^+ + H_2O$ <ul style="list-style-type: none"> ◇ The oxygen consumption is proportional to a nitrification rate and a function of the DO and ammonium concentration.
Denitrification ⁷	OXY (NO3)	$NO_3^- + H^+ \rightarrow 0.5N_2 + 1.25O_2 + 0.5H_2O$ <ul style="list-style-type: none"> ◇ The oxygen production is proportional to a denitrification rate and a function of the DO and nitrate concentration.
Mineralization in the water column	OXY CBOD5 CBODu NBOD5 NBODu COD	<ul style="list-style-type: none"> ◇ The oxygen consumption and the mineralization of BOD/COD is proportional to a mineralization rate. ◇ Optionally an age function can be applied to the mineralization rate of BOD/COD to take into account the reduced degradability of organic matter as it ages.
Mineralization in the sediment	OXY SOD	<ul style="list-style-type: none"> ◇ The oxygen consumption and the mineralization of SOD is proportional to a mineralization rate.
Settling ⁵	CBOD5 CBODu NBOD5 NBODu COD SOD	<ul style="list-style-type: none"> ◇ Settling is proportional to a first order settling velocity (in m/d). ◇ Settling occurs when the actual shear stress is lower than the user-defined critical shear stress for sedimentation. ◇ The actual shear stress is a function of flow velocity and waves. Artificial disturbances such as ships can be added as well. ◇ Each particulate fraction has its own critical shear stress for sedimentation. ◇ Settled matter may be allocated to both the first and the second layer, as indicated by a user-defined fraction (the "buffer" model, (Van Kessel <i>et al.</i>, 2011)) ◇ All fractions in the water column are combined into SOD after settling to the sediment.

Remarks:³For process equations refer to [section 6.7](#)

- ◇ All reaction rates are temperature dependent ([section 6.3](#)).
- ◇ A daily variation of algae can be described by constraining the gross primary production to the daylight period. Algal respiration will take place 24 hours per day. As a result dissolved oxygen will be produced during daylight and consumed during the night.
- ◇ In D-Water Quality the consumption of dissolved oxygen may lead to a negative dissolved oxygen concentration, i.e. the dissolved oxygen concentration is not restricted to positive values. The reason for this is that some reduced substances (e.g. sulphides, iron(II), methane) may not be included in your model, but would oxidise rapidly when coming into contact with dissolved oxygen. Negative dissolved oxygen concentrations should therefore be considered as (negative) oxygen equivalents. Optionally, negative oxygen concentrations can be prevented by letting the mineralization rate depend on dissolved oxygen concentration (e.g. if DO < 0.1 mg/l, then mineralization rate = 0 d⁻¹), but this implies a biased degradation rate.

6.5.3 Process equations

Reaeration

The reaeration rate is a linear function of the difference between the saturation and actual DO concentration according to:

$$R_{rear} = k_{lrear} \times (C_{oxs} - C_{ox}) / H$$

$$k_{lrear} = \left(\frac{a \times v^b}{H^c} \right) + (d \times W^2)$$

$$C_{oxs} = f(T, C_{cl}) = f(T, SAL)$$

with:

a, b, c, d	coefficients with different values for eleven reaeration options
C_{cl}	chloride concentration [gCl m ⁻³]
C_{ox}	actual dissolved oxygen concentration [gO ₂ m ⁻³]
C_{oxs}	saturation dissolved oxygen concentration [gO ₂ m ⁻³]
H	depth of the water column [m]
k_{lrear}	reaeration transfer coefficient in water [d ⁻¹]
R_{rear}	reaeration rate [gO ₂ m ⁻³ d ⁻¹]
SAL	salinity [kg m ⁻³]
T	water temperature [°C]
v	flow velocity [m s ⁻¹]
W	wind speed at 10 m height [m s ⁻¹]

Depending on the reaeration option the transfer coefficient is only dependent on the stream velocity or the wind speed, or dependent on both. A host of alternative formulations is available. In addition to the water temperature the saturation concentration is a function of either the chloride concentration or the salinity (two options available).

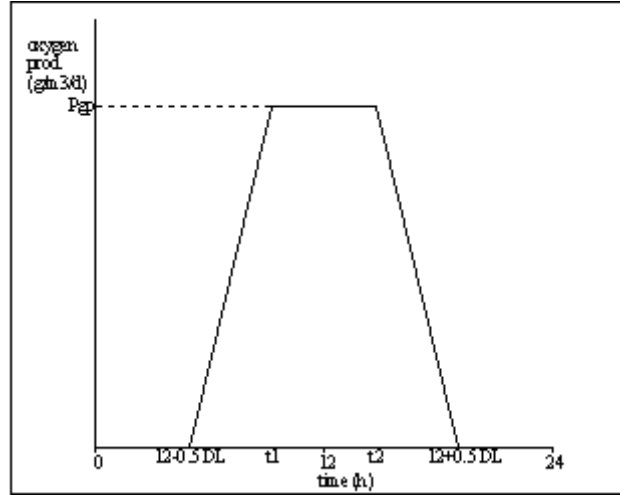


Figure 6.4: The distribution of gross primary production over a day

Diurnal variation of production

The phytoplankton models implemented in D-Water Quality are subjected to daily averaged forcing functions. However, in reality the gross primary production of phytoplankton is constrained to daytime, whereas respiration consumes oxygen all day. The resulting diurnal variation of the dissolved oxygen concentration follows from the production distribution over a day as displayed in Figure 6.4. The shape of the production curve depends on day length (DL) and the times (t_1) and (t_2), which define the period of the maximum production during a day $R_{gp_{max}}$. The maximal primary production in a day follows from:

$$R_{gp_{max}} = \frac{48 \times R_{gpa}}{t_2 - t_1 + DL}$$

with:

DL	day length [hr]
R_{gpa}	daily average gross primary production rate [$\text{gO}_2 \text{ m}^{-3} \text{ d}^{-1}$]
$R_{gp_{max}}$	maximal gross primary production rate during a day [$\text{gO}_2 \text{ m}^{-3} \text{ d}^{-1}$]
t_1	time at which the maximal production is reached [h]
t_2	time at which the production starts to decrease [h]

Mineralization

The mineralization rate of all BOD/COD-components depends on the age of the organic matter, provided that BOD and COD are simulated simultaneously. By default the function of the age function (f_{age}) is 1.0. The mineralization rate is described with first-order kinetics according to:

$$R_{min} = f_{age} \times k_{min} \times Cx \quad (6.6)$$

$$f_{age} = f_{age_{min}} + (f_{age_{max}} - f_{age_{min}}) \times e^{f(AI)} \quad (6.7)$$

$$AI = \frac{COD}{BOD5} \quad (6.8)$$

with:

AI	index for the age of organic matter [-]
Cx	concentration of a BOD/COD-component [$\text{gO}_2 \text{ m}^{-3}$]
$BOD5$	concentration of total CBOD5 [$\text{gO}_2 \text{ m}^{-3}$]

COD	concentration of total COD [$\text{gO}_2 \text{ m}^{-3}$]
f_{age}	attenuation function for age [-]
k_{\min}	first-order kinetic constant [d^{-1}]
R_{\min}	mineralization rate of a BOD/COD-component [$\text{gO}_2 \text{ m}^{-3} \text{ d}^{-1}$]

The Sediment Oxygen Demand (SOD) has been formulated as the sum of a zero-order and a first-order process, allowing the specification of a background sediment oxygen demand. Two options are available for the mineralization rate, one of which takes into account the escape of methane to the atmosphere. The mineralization rate according to option 2 is calculated with:

$$Rsod = (1 - f_{ch4}) \times \left(\frac{k0sod}{H} + \frac{ksod \times SOD}{V} \right)$$

with:

SOD	quantity of potential sediment oxygen demand [gO_2]
f_{ch4}	fraction of organic matter escaped as methane [-]
$k0sod$	constant "background" sediment oxygen demand [$\text{gO}_2 \text{ m}^{-2} \text{ d}^{-1}$]
$ksod$	first-order kinetic constant [d^{-1}]
H	depth of the water column [m]
$Rsod$	sediment oxygen demand [$\text{gO}_2 \text{ m}^{-3} \text{ d}^{-1}$]
V	volume of the water compartment [m^3]

Positive DO

The concentration of dissolved oxygen (DO) may become negative in D-Water Quality. Positive parameter DO is calculated for presentation purposes with:

$$DO = \max(Cox, 0.0)$$

with:

DO	dissolved oxygen concentration [$\text{gO}_2 \text{ m}^{-3}$]
Cox	equivalent dissolved oxygen concentration, substance, OXY [$\text{gO}_2 \text{ m}^{-3}$]

Minimal DO

The minimal DO concentration in a day resulting from the diurnal variation of primary production is computed according to:

$$Cox_{\min} = f(Cox, Rnp, Rrsp, DL)$$

with:

Cox	average dissolved oxygen concentration [$\text{gO}_2 \text{ m}^{-3}$]
Cox_{\min}	minimal dissolved oxygen concentration in a day [$\text{gO}_2 \text{ m}^{-3}$]
DL	daylength [hr]
Rnp	total net primary production rate [$\text{gC m}^{-3} \text{ d}^{-1}$]
$Rrsp$	total algae respiration rate [$\text{gC m}^{-3} \text{ d}^{-1}$]

6.6 Suspended sediment, sedimentation and erosion

6.6.1 Concepts

Sediment is particulate material, formed by the physical and chemical desintegration of rocks from the earth's crust (i.e. inorganic) and by various biological processes (i.e. organic). The sediment carried by natural waters contains a mixture of inorganic and organic components with can be classified according to the various grain sizes:

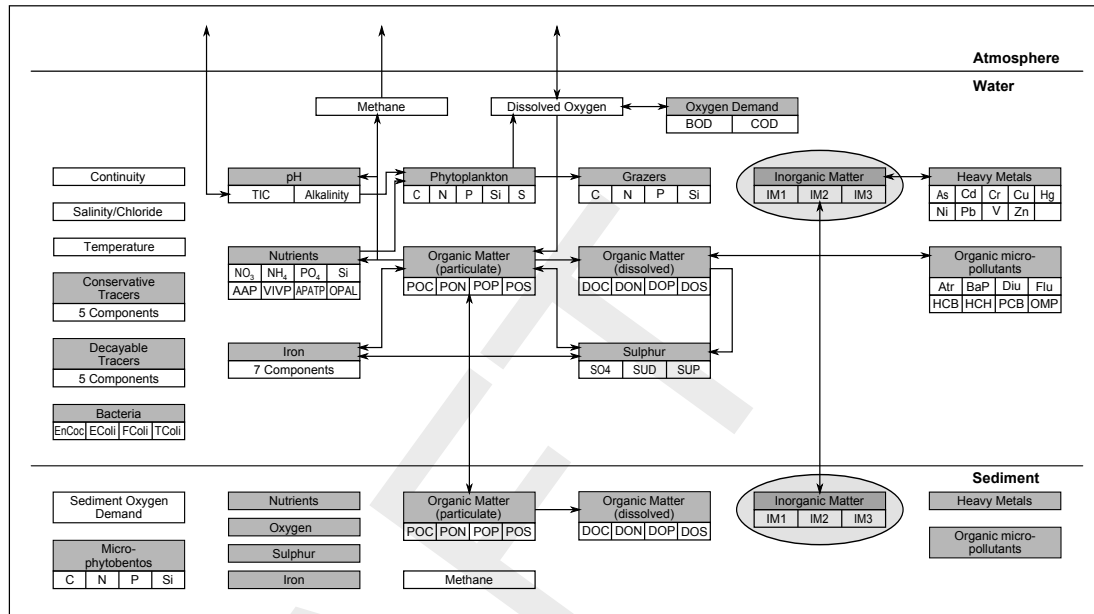


Figure 6.5: Overview of substances. Suspended sediment, sedimentation and erosion

- | | |
|---------------------|-------------------------|
| 1 Gravel | : >2 mm |
| 2 Sand | : 0.06 mm - 2 mm |
| 3 Silt | : 0.004 mm - 0.06 mm |
| 4 Clay | : <0.004 mm |
| 5 Organic particles | : up to several μ m |

The very fine organic particles of living and dead algae and the silt and clay fractions can be carried as colloidal suspension for which electrochemical forces play a predominant role. Considering the large adsorbing capacities, the fine fraction is characterised as cohesive sediment. Since flocculation and adsorbing capacities are of minor importance for larger particles, they are classified as non-cohesive sediment. In principal all particulate components are subject to settling and resuspension to and from the bed.

Fine grained (cohesive) particulate sediments

All fine grained suspended matter which range in size from several microns up to about 70 microns and are easily brought into suspension. The behaviour of this fine grained suspended matter plays an important role in water quality. First, turbidity and its effect on the under-water light climate is an important environmental condition for algae growth. The presence of suspended sediment increases the attenuation of light in the water column which leads to an inhibition of photosynthetic activity and hence, a reduction in primary production. Secondly, the fate of contaminants in waters is closely related to suspended solids due to their large adsorbing capacities. Like dissolved matter, the sediment is transported by advection and by turbulent motion. In addition, the fate of the fine grained suspended sediments is determined by settling and deposition, as well as by bed processes, e.g. consolidation, bioturbation and resuspension. The sedimentation and erosion processes originate from the Partheniades-Krone concept (Partheniades, 1962; Krone, 1962). In this concept, the bottom shear stress plays an essential role in defining whether or not sedimentation of suspended particles or erosion of bed material will occur. Deposition takes place when the bottom shear drops below a critical value. On the other hand erosion occurs when the bottom shear exceeds a critical value.

Suspended matter in the water column is subject to settling onto the sediment and the fractions in the sediment are subject to erosion (or resuspension). In turn the sediment is subject to processes known as 'burial' and 'digging' that transfer the sediment matter to and from a deeper layer.

Coarse grained (non-cohesive) sediment

Particle sizes of non-cohesive material are larger than those of cohesive sediment, and are in the order of 100 µm and more (sandy). The behaviour of this sandy sediment transport is of major importance in coastal engineering problems related to morphological changes. The transport of sediment particles can be in the form of bed-load and suspended load, depending on the size of the bed material and the local instantaneous flow conditions (Van Rijn, 1993). The transport of particles via rolling, sliding and jumping (saltating) is called bed load transport and this motion is exclusively determined by the effective bed shear which is assumed to be dominated by gravity forces. The bed load transport takes places in a thin layer above the surface of the sediment. The suspended load is that part of the total load that is moving without continuous contact with the bed as a result of the agitation of fluid turbulence. The suspended sediment is only affected by the friction of the grains themselves in the water. Whether there is merely a bed load or a suspended load depends primarily on the intensity of the water movement. There is a critical velocity below which no movement occurs. If the velocity increases, bottom transport is initiated to develop ripples and dunes. At higher velocities, sediment grains come into suspension and suspended loads starts.

The transport rate of non-cohesive sediment is determined by the local instantaneous flow conditions. This assumption is commonly assumed for bed load transport. For suspended transport it implies that the time and length scale of the flow variation are much larger than the adaptation time and adaptation length of the sediment concentration respectively. The transport of such sediment is not related to the flow field in the same way as for dissolved substances and hence no dispersion or diffusion is applied.

There are many transport formulation in literature to describe the bed and suspended loads transport. In D-Water Quality the transport formulation for the total load of Engelund and Hansen (1967) is implemented since this formula is relatively simple and has shown good performance in numerous field and laboratory experiments.

6.6.2 Modelling framework

The (inorganic) substances that can be modelled in the D-Water Quality in relation to particulate matter are:

Name	Description	Unit
IM1	suspended inorganic matter fraction 1	g/m ³
IM2	suspended inorganic matter fraction 2	g/m ³
IM3	suspended inorganic matter fraction 3	g/m ³
IM1S1	inorganic matter fraction 1 in bed layer 1	g
IM2S1	inorganic matter fraction 2 in bed layer 1	g
IM3S1	inorganic matter fraction 3 in bed layer 1	g
IM1S2	inorganic matter fraction 1 in bed layer 2	g
IM2S2	inorganic matter fraction 2 in bed layer 2	g
IM3S2	inorganic matter fraction 3 in bed layer 2	g

Remark:

- ◇ There are (living and dead) particulate organic substances as well (DetC, OOC, POC1, Algae, etc.). Also adsorbed phosphate can be simulated as a particulate substance. These substances undergo the same processes for sedimentation, erosion, burial and digging. However, they are not mentioned explicitly in the remainder of this chapter.

The mass balances for particulate (suspended) matter in the water column (c_w) and particulate matter in the sediment (c_b) is given in [Equation \(6.9\)](#) and [Equation \(6.10\)](#) respectively.

$$\frac{\Delta c_w}{\Delta t} = \text{loads} + \text{transport} - \text{settling} + \text{resuspension} \quad (6.9)$$

$$\frac{\Delta c_b}{\Delta t} = \text{loads} + \text{settling} - \text{resuspension} - \text{burial} + \text{digging} \quad (6.10)$$

Brief description and relevant notes of processes:

Process	Substances	Comments
Settling / sedimentation	IM1 IM2 IM3 (all particulates)	<ul style="list-style-type: none"> ◇ Settling is proportional to a first order settling velocity (in m/d). ◇ Settling occurs when the actual shear stress is lower than the user-defined critical shear stress for sedimentation. ◇ The actual shear stress is a function of flow velocity and waves. Artificial disturbances such as ships can be added as well. ◇ Each particulate fraction has its own critical shear stress for sedimentation. ◇ Settled matter may be allocated to both the first and the second layer, as indicated by a user-defined fraction (the 'buffer' model, (Van Kessel et al., 2011)).
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Process	Substances	Comments
Resuspension	IM1S1/IM1S2 IM2S1/IM2S2 IM3S1/IM3S2 (all particulates)	<ul style="list-style-type: none"> ◇ Resuspension takes places with a zero-order rate (in g/m²/d) and is proportional to a probability function. ◇ Resuspension takes place when the actual shear stress is higher than the critical shear stress for resuspension. ◇ The sediment layers S1 and S2 each have a critical shear stress for resuspension. The critical shear stress for resuspension is valid for all particulate fractions in the sediment layer. ◇ The resuspension rate of the individual particulate fractions in the sediment layer is proportional to its weight fraction. ◇ If the "buffer" model, ((Van Kessel et al., 2011)) is used, the total resuspension flux from both the fluff layer (S1) and the buffer layer (S2) is calculated first for the inorganic matter fractions IM1, IM2 and IM3 (Section 6.6) and increased in proportion to the organic content (measured by DM relative to TIM) of these two layers. The net result is that the share of all sediment substances that resuspends equals the share of IM1+IM2+IM3 that resuspends. ◇ The resuspension may occur from the second layer via Van Rijn pick-up.
Burial	IM1S1/IM1S2 IM2S1/IM2S2 IM3S1/IM3S2 (all particulates)	<ul style="list-style-type: none"> ◇ Burial is the downward movement of particulates in the sediment. Sediment layers can have either a fixed or a variable layer thickness. ◇ When considered independent of the thickness of a sediment layer, burial can consist of a zero-order and a first-order term. ◇ When the prescribed layer thickness is exceeded, exceedance burial can take place. ◇ Combined burial takes places for all particulate fraction. ◇ The burial rate of the individual particulate fractions in the sediment layer is proportional to its weight fraction.
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Process	Substances	Comments
Digging	IM1S1/IM1S2 IM2S1/IM2S2 IM3S1/IM3S2 (all particulates)	<ul style="list-style-type: none"> ◇ Digging is the upward movement of particulates in the sediment. Sediment layers can have either a fixed or a variable layer thickness. ◇ When considered independent of the thickness of a sediment layer, digging can consist of a zero-order and a first-order term. ◇ When the prescribed layer thickness is not met, replenishment digging can take place. ◇ Combined digging takes places for all particulate fraction. ◇ The digging rate of the individual particulate fractions in the sediment layer is proportional to its weight fraction.

6.6.3 Processes

Sedimentation of suspended fine-grained particulate matter

A characteristic feature of fine sediments is the ability to form aggregates of flocs that settle to the bottom. Whether a particle will settle to the bottom depends upon its size and density and the chemical conditions of the surrounding water system. Sedimentation is the process describing the settling of particles. This deposition process is described with the formulation by [Krone \(1962\)](#). Various laboratory and field measurements show that the suspended matter concentration strongly influences the aggregation process and thereby the settling velocities of the aggregates. Strong flocs are denser and have larger settling velocities. The aggregation of flocs strongly depends on the chemical and physical properties of the sediment, salinity and turbulence. At high sediment concentrations (several g/l) the particles hinder each other, resulting in a decrease of the settling velocity. Turbulence is an important parameter because it affects the flocculation and therefore the settling velocity in two opposing ways. On the one hand an increase in turbulence will increase the collisions between particles, resulting in larger flocs with high settling velocities. On the other hand, it results in turbulent shear stresses which can break up the flocs and decrease the settling velocity. At low suspended concentrations however, flocculation processes are so low, that the floc size, hence settling velocity does not vary over the depth. So the floc formation and floc break-up processes will only play a role in the sedimentation process at high-concentrated conditions ([Winterwerp, 2002](#)).

When applying the burial/digging method, the rate of downward mass transport (deposition) is equal to the product of the near-bed velocity, the concentration and the probability that a settling particle becomes attached to the sea bed. The deposition (i.e. sedimentation flux) ([Krone, 1962](#)) is given by:

$$D = w_s \cdot C \cdot \left(1 - \frac{\tau_b}{\tau_c}\right)$$

with:

D deposition flux of suspended matter [$\text{g m}^{-2} \text{d}^{-1}$]

w_s	settling velocity of suspended matter [m d^{-1}]
C	concentration of suspended matter near the bed [g m^{-3}]
τ_b	bottom shear stress [Pa]
τ_d	critical shear stress for deposition [Pa]

Sedimentation with this method always results in an increase of sediment in the upper sediment bed layer. In the implemented sedimentation process it is assumed that there is no correlation between the various sediment components which means that each of the particulate fractions can settle independently.

When applying the buffer model deposition towards layer S1 and S2 is determined by both the settling velocity w_s , and a deposition flux factor ($\alpha < 1$) that distributes the flux to the fluff and buffer layer. A critical shear stress for sedimentation is not applied and should be set to 0:

$$D_1 = (1 - \alpha)w_s C$$

$$D_2 = \alpha w_s C$$

with:

D_1	deposition flux to layer S1 [$\text{g m}^{-2} \text{d}^{-1}$]
D_2	deposition flux to layer S2 [$\text{g m}^{-2} \text{d}^{-1}$]
α	fraction of the deposition flux allocated to layer S2 [-]

Erosion of particulate fine-grained matter

Erosion of bed material occurs when the bed shear forces exceed the resistance of the bed sediment. The resistance of the bed is characterised by a certain critical erosive strength (bottom shear stress). This critical stress is determined by several factors, such as, the chemical composition of the bed material, particle size distribution and bioturbation. Erosion of sediment is induced by the bed stress due to tidal and wind-induced advective flows and surface waves. The erosion is directly proportional to the excess of the applied shear stress over the critical erosive bottom shear stress. The formula for erosion of homogeneous beds is based on [Partheniades \(1962\)](#). The erosion flux is limited by the available amount of sediment on the sea bed.

The erosion of bed material is given by:

$$E = M \left(\frac{\tau_b}{\tau_c} - 1 \right)$$

with:

E	erosion rate [$\text{g m}^{-2} \text{d}^{-1}$]
M	first order erosion rate [$\text{g m}^{-2} \text{d}^{-1}$]
τ_b	bed shear stress [Pa]
τ_c	critical shear stress for erosion [Pa]

The values of M and τ strongly dependent on the sediment properties and environmental parameters. The amount of eroded dry matter is added to the mass in the water column. In D-Water Quality a variable sediment layer or a fixed sediment layer can be selected. For the variable-layer option, the erosion flux is limited based on the available amount of sediment in a sediment layer. The flux is unlimited if the fixed layer option is applied. As long as mass is available in the upper sediment layer, resuspension takes place from that layer only. If the upper sediment layer is completely eroded, then resuspension takes place from the lower sediment layer.

In the buffer model formulation, Resuspension E_1 of each fraction out of the fluff layer (S1) is proportional to the excess shear stress times a grain size dependent first-order rate (V_{Res}) until a certain saturation concentration in the bed is attained beyond which a uniform zero-order rate (Z_{Res}) applies. The coarse and fine fractions may have a different critical shear stress for resuspension (τ_{cr}). The zero-order formulations are based on (Partheniades, 1962), the first order expression is based on (Van Kessel *et al.*, 2011). The process is implemented for all three sediment fractions IMi.

For the resuspension flux E_2 from the buffer layer (S2), a (Van Rijn, 1993) type of pickup formulation is applied, with Van Rijn's empirical power of the excess stress of 1.5. The fines are only detrained from this layer when the shear stress exceeds the mobilization threshold (Shields stress, τ_{Sh}) for the sand amongst which the fines are stored. In summary, the erosion fluxes are:

$$E_1 = \min(Z_{res}, V_{res} f_{IMiS1} M) \left(\frac{\tau_b}{\tau_{\alpha, S1}} - 1 \right)$$

$$E_2 = f_{IMiS2} F_{resPUP} \rho_s ((s-1)gD_{50})^{0.5} D_*^{0.3} \left(\frac{\tau_b}{\tau_{Sh}} - 1 \right)$$

$$D_* = D_{50} ((s-1)g/\nu^2)^{1/3}$$

$$s = \rho_s / \rho_w$$

with:

D_{50}	median grain size (diameter) [m]
D_*	reduced grain size [-]
E_1	resuspension flux of the i'th SPM fraction (IMiS1) from layer S1 [$\text{g m}^{-2} \text{d}^{-1}$]
E_2	resuspension flux of the i'th SPM fraction (IMiS2) from layer S2 [$\text{g m}^{-2} \text{d}^{-1}$]
F_{resPUP}	Van Rijn (1993) pickup factor from buffer layer [-]
f_{IMiS1}	the i'th fraction of SPM in layer S1 [-]
f_{IMiS2}	the i'th fraction of SPM in layer S2 [-]
Z_{res}	zeroth-order resuspension rate from layer S1 [$\text{g m}^{-2} \text{d}^{-1}$]
ρ_s	density of the sediment [kg m^{-3}]
ρ_w	density of water [kg m^{-3}]
$\tau_{\alpha, S1}$	critical bed shear stress for layer S1 [Pa]
τ_{Sh}	Shields shear stress for layer S2 [Pa]

Total Bed shear stress

The bed shear stress is an essential quantity that directly influences the sedimentation and erosion rates. It depends on the flow (currents) and the wind generated surface waves. For the sedimentation/erosion processes it is assumed that the bed stresses due to flow (τ_{flow}) and waves (τ_w) are additive. In addition, a third shear stress component can be defined (τ_{ship}) to be representative for the bed shear stresses due to shipping or fishing activities.

$$\tau = \tau_{flow} + \tau_w + \tau_{ship} \quad (6.11)$$

1. Bed shear stress to currents (τ_{flow})

The effects of the hydrodynamic forcing on the sediments take place primarily through the friction they exert on the sea bed shear stress τ_{flow} . This shear stress is described by the following formulae:

In case of depth averaged (2D) flow:

$$\tau_{flow} = \frac{\rho \cdot g}{C_{2D}^2} \cdot u^2 \quad \text{or} \quad \rho \cdot u_*^2 \quad (6.12)$$

For hydraulic rough flows, the 2D Chezy coefficient (C_{2D}) can be determined according to Manning's formulation or the White Colebrook formulation:

$$\text{Manning: } C_{2D} = \frac{\sqrt[6]{h}}{n}$$

$$\text{White Colebrook: } C_{2D} = 18 \cdot 10 \log \left(\frac{12h}{k_s} \right)$$

In case of three dimensional flow, the logarithmic velocity current profile can be written as:

$$u(z) = \frac{u_*}{\kappa} \ln \left(\frac{z}{z_0} \right) \quad (6.13)$$

Averaging over the depth yields:

$$\bar{u} = \frac{u_*}{\kappa} \left[\ln \left(\frac{H}{z_0} \right) - 1 \right] \quad (6.14)$$

where:

$$u_* = \sqrt{g} \frac{\bar{u}}{C_{2D}} \quad (6.15)$$

Substitution of Equation (6.15) in Equation (6.14) results in an expression of z_0 :

$$z_0 = H e^{-\left(1 + \frac{\kappa \cdot C_{2D}}{\sqrt{g}}\right)} \quad (6.16)$$

Now, assuming equality of bed stresses for 2D and 3D simulations, the shear stress and the Chezy coefficient for three-dimensional flows can be written as follows:

$$\tau_{flow} = \frac{g \rho_l}{C_{3D}^2} \vec{u}_b |\vec{u}_b| \quad (6.17)$$

$$C_{3D} = \frac{\sqrt{g}}{\kappa} \ln \left(1 + \frac{h_b/2}{z_0} \right) \quad (6.18)$$

with:

g	acceleration of gravity [m/s ²]
C_{3D}	3D Chézy coefficient [m ^{1/2} /s]
C_{2D}	2D Chézy coefficient [m ^{1/2} /s]
u_b	velocity at bed layer [m/s]
u_*	bed-shear velocity [m/s]
u	depth averaged horizontal velocity [m/s]
n	Manning coefficient [m ^{-1/3} s ¹]
H	total water depth [m]
h_b	thickness of bed layer [m]
κ	constant of Von Kármán (0.4) [-]

$k_0 = 0.24$	$k_1 = 0.015$	$k_2 = 0.0345$	$k_3 = 0.710$	$k_4 = 0.855$
$m_0 = 2\pi$	$m_1 = 0.45$	$m_2 = 0.37$	$m_3 = 0.763$	$m_4 = 0.365$

k_s Nikuradse roughness ($= 30z_0$) [m]
 z_0 roughness height of the bed (i.e. zero velocity level) [m]

The Nikuradse roughness k_s is related to the roughness length z_0 by the relationship $k_s = 30z_0$ for hydrodynamic rough flows. At height $z = z_0$ above the bed, the velocity is zero. Several relationships between k_s and grain size have been proposed, with one of the most widely used being:

$$k_s = 2.5D_{50}$$

with D_{50} being the median grain size [m^{-1}].

2. Bed shear stress to waves (τ_w)

Surface waves are caused by wind stress on the water surface. The magnitude of the waves depends on the wind conditions, wind duration, water depth and bottom friction. Wave fields are commonly described by the significant wave height, significant wave period and wave length. The magnitude of a equilibrium wave field can be estimated with the formulae by [Groen and Dorrestein \(1976\)](#) for wind-generated waves. The wave growth is limited by the water depth according to an analysis given by [Nelson \(1983\)](#). The wave-induced bed shear stress is computed after [Soulsby \(1997\)](#) and [Van Rijn \(1993\)](#), using linear wave theory.

Relevant wave parameters for wave height and period of wind-generated waves are made non-dimensional with the wind speed at 10 m height U_{10} and the gravitational acceleration g :

$$\text{water depth: } h_* = \frac{gh}{U_{10}^2} \quad (6.19)$$

$$\text{fetch: } F_* = \frac{gF}{U_{10}^2} \quad (6.20)$$

$$\text{wave height: } H_* = \frac{gH}{U_{10}^2} \quad (6.21)$$

$$\text{wave period: } T_* = \frac{gT}{U_{10}} \quad (6.22)$$

Significant wave height and period as a function of water depth and fetch for unlimited wind duration are given by [Groen and Dorrestein \(1976\)](#):

$$H_* = k_0 \tanh(k_3 h_*^{m_3}) \tanh\left(\frac{k_1 F_*^{m_1}}{\tanh(k_3 h_*^{m_3})}\right)$$

$$T_* = m_0 \tanh(k_4 h_*^{m_4}) \tanh\left(\frac{k_2 F_*^{m_2}}{\tanh(k_4 h_*^{m_4})}\right)$$

with the coefficients k_n and m_n :

The wave height is limited to $0.55h$ (Nelson, 1983); when the wave height computed with would exceed this criterion, the wave height is kept constant at $H = 0.55h$. It is assumed that also the wave period stops growing, and T is kept at the value attained when H exceeds $0.55h$. The wavelength L follows from linear wave theory and is given in the following implicit formula that has to be solved iteratively:

$$T = \sqrt{\frac{2\pi}{g} L \coth\left(\frac{2\pi h}{L}\right)}$$

The amplitude of the wave orbital velocity (U_{orb}) just above the bed follows from linear wave theory:

$$U_{orb} = \frac{\pi H}{T \sinh(2\pi h/L)}$$

Waves induce a vertical circular movement (orbital velocity) which decreases with depth. The waves exert friction forces at the bed during propagation. The magnitude of the time-averaged wave-induced bed shear stress follows from Van Rijn (1993):

$$\tau_w = \frac{1}{4} \rho f_w U_{orb}^2$$

where f_w is a wave friction factor.

For rough turbulent flows a number of formulae have been proposed for the friction factor. In D-Water Quality two commonly used formulation have been implemented:

1 Tamminga (1987)

$$f_w = 0.16 \sqrt{\frac{k_s}{U_{orb} T/2\pi}}$$

2 Swart (1974)

$$f_w = \begin{cases} 0.3 & \text{for } r \leq \pi/2 \\ 0.00251 \exp(5.21 r^{-0.19}) & \text{for } r > \pi/2 \end{cases}$$

3 Soulsby (1997)

$$f_w = 0.237 r^{-0.52}$$

where:

$$r = \frac{A}{k_s}$$

r	relative roughness height [-]
A	semi-orbital excursion $A = U_{orb} T/2\pi$ [m]
k_s	Nikuradse roughness [m]

Burial and Digging

In addition to the described water-bed exchange processes, particulate components in the bed layer can be transferred downward from one sediment layer to an underlying layer (i.e. burial). This process can be defined either by a zero-order or a first order burial rate. The sediment layer is considered to be homogeneous, therefore the composition of the sediment being buried is the same as that of the (overlying) sediment layer. Sediment can also be transferred upward to one sediment layer from an underlying layer in a process known as 'digging'. The composition of the sediment being transported upwards is the same as that of the (underlying) sediment layer.

Non-cohesive total bed load transport

A sediment transport formula is an algebraic equation relating the sediment rate with the flow parameters. One of the well known formulae is that of [Engelund and Hansen \(1967\)](#):

$$S = \frac{0.05 u^2 u_*^3}{D g^2 \Delta \rho^2}$$

$$\Delta \rho = \frac{\rho_s - \rho}{\rho}$$

where:

S	sediment transport rate [m ² /s]
u	depth averaged flow velocity [m/s]
u_*	bed shear stress velocity [m/s]
D	grain size of sediment [m]
g	gravity [m/s ²]
$\Delta \rho$	relative density of sediment [-]

Non-cohesive sediment is modelled as an inactive substance to prevent the transport algorithms in D-Water Quality from acting on this substance. The horizontal transport rate results in a change of the amount of sediment present in the bed. This change is expressed as a change in the thickness of the layer of non-cohesive sediment. There is no feed-back of the bed level change towards the hydrodynamics.

Remark:

- ◇ The sedimentation process is described with the classical formulation by [Krone \(1962\)](#). In this formulation the rate of downward mass transport (deposition) is equal to the product of the near-bed velocity, the concentration and the probability that a settling particle becomes attached to the sea bed (depending on the critical shear stress of deposition). A re-analysis of the experiments of Krone by [Winterwerp and Van Kesteren \(2004\)](#) revealed however that the so-called critical shear stress for deposition does not exist. In fact, it represents the critical shear stress for erosion of freshly deposited sediment. Hence, the classical Krone formulation contains both a deposition and an erosion term. This means that in common engineering practise, in which the water-bed exchange processes are described with a combination of the Krone's deposition formula and Partheniades' erosion formula is basically wrong. It is therefore proposed to model the sedimentation flux for applications at low-concentrated cohesive sediment simply by the deposition flux (D) itself:

$$D = w_s c$$

6.7 Nutrients, detrital organic matter and electron-acceptors

6.7.1 Concepts

The major elements that form organic matter are carbon (C), nitrogen (N), phosphorus (P), sulphur (S), oxygen (O) and hydrogen (H). Many other elements (Fe, Ca, K, etc.) are incorporated in minor quantities, but are not included in the D-Water Quality modelling framework with respect to organic components. A special place is reserved for silicon (Si). As certain types of phytoplankton use silicon to construct a skeletal structure, silicon is usually considered as a nutrient as well, although it is not incorporated in organic matter but in silicate minerals, mostly opal (SiO_2).

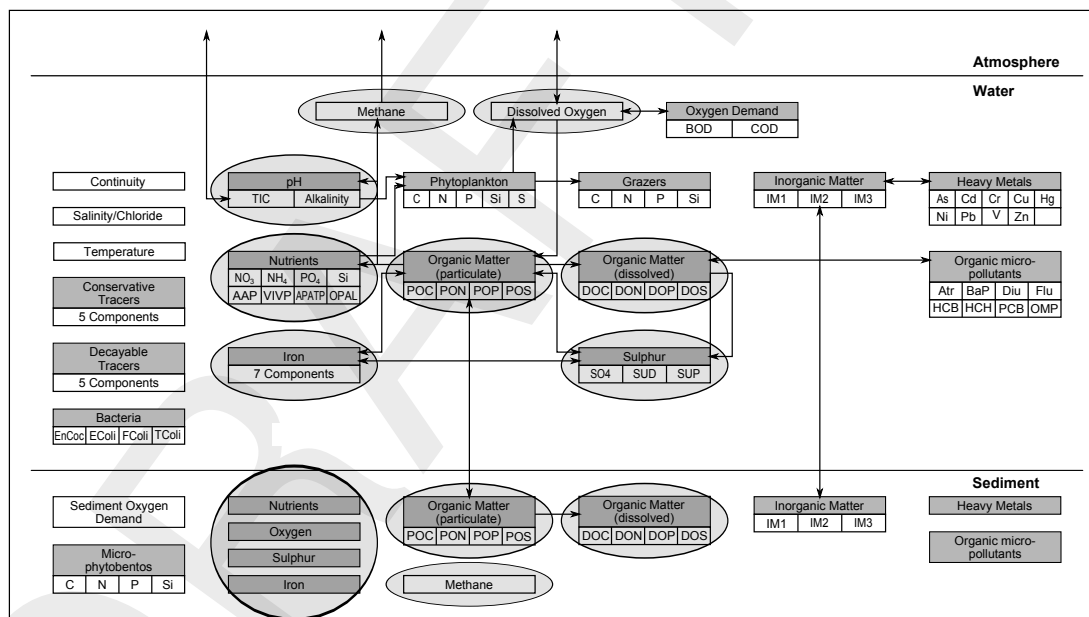


Figure 6.6: Overview of substances. Nutrients, detrital organic matter and electron-acceptors

The nutrient cycle has four major pools: dissolved inorganic nutrients, particulate inorganic nutrients, living organic matter (biomass) and detrital organic matter. Dissolved inorganic nutrients and carbon dioxide are taken up by primary producers into their biomass⁴. When we do not consider the food chain in which biomass can be taken up by ever higher trophic levels, nutrients become available when primary producers die. Part of the nutrients are released as dissolved inorganic nutrients again in a process that is called autolysis. The other part is released as detrital organic matter (or as Opal), which can be dissolved or particulate. Finally microbial decomposition of detrital organic matter releases the nutrients and carbon back to their dissolved inorganic form. Electron-acceptors such as oxygen, nitrate, iron(III) and sulphate are consumed for the decomposition of organic matter. Nitrate and sulphate are both nutrients and electron-acceptors. Because carbon dioxide and alkalinity are consumed in primary production and produced at the mineralization of organic matter these processes affect the pH.

Particulate organic matter can settle to the sediment as a result of which nutrients can be trapped in the sediment. Decomposition of organic matter and dissolution of opal silicate will continue there and (eventually) nutrients are released back to the water column. Apart from carbon dioxide, methane is produced in the degradation process. Substantial quantities

⁴For a detailed description of primary producers refer to [section 6.8](#).

of the nutrients may be nitrified, denitrified, adsorbed or precipitated in the sediment⁵. Also, primary producers living on the sediment (microphytobenthos) fix dissolved inorganic nutrients in biomass in the sediment.

6.7.2 Modelling framework

The substances that can be modelled in D-Water Quality in relation to nutrients and detrital organic matter in the water column are:

Name of D-Water Quality substance	Description	Unit
<i>Inorganic dissolved nutrients</i>		
NO3	Nitrate	gN/m ³
NH4	Ammonium	gN/m ³
PO4	Ortho-phosphate	gP/m ³
Si	Silicon	gSi/m ³
SO4	Sulphate	gS/m ³
TIC	Total dissolved inorganic carbon	gC/m ³
(Alka)	Alkalinity, only needed for pH simulation	gHCO ₃ ⁻ /m ³
<i>Inorganic particulate nutrients</i>		
AAP	Adsorbed phosphate	gP/m ³
VIVP	Vivianite like P (Fe ₃ (PO ₄) ₂)	gP/m ³
APATP	Apatite like P (Ca(CO ₃) _n (PO ₄) _m)	gP/m ³
Opal	Opal silicate (SiO ₂)	gSi/m ³
SUP	Precipitated sulphide	gS/m ³
<i>Particulate detrital organic matter</i>		
POC1	Particulate Organic Carbon fraction 1	gC/m ³
POC2	Particulate Organic Carbon fraction 2	gC/m ³
POC3	Particulate Organic Carbon fraction 3	gC/m ³
POC4	Particulate Organic Carbon fraction 4	gC/m ³
POC5	Particulate Organic Carbon fraction 5	gC/m ³
PON1	Particulate Organic Nitrogen fraction 1	gN/m ³
PON2	Particulate Organic Nitrogen fraction 2	gN/m ³
PON3	Particulate Organic Nitrogen fraction 3	gN/m ³
PON4	Particulate Organic Nitrogen fraction 4	gN/m ³
PON5	Particulate Organic Nitrogen fraction 5	gN/m ³
POP1	Particulate Organic Phosphorus fraction 1	gP/m ³
POP2	Particulate Organic Phosphorus fraction 2	gP/m ³
POP3	Particulate Organic Phosphorus fraction 3	gP/m ³

⁵For a detailed description of sediment processes refer to [section 6.11](#).

Name of D-Water substance	Description	Unit
POP4	Particulate Organic Phosphorus fraction 4	gP/m ³
POP5	Particulate Organic Phosphorus fraction 5	gP/m ³
POS1	Particulate Organic Sulphur fraction 1	gS/m ³
POS2	Particulate Organic Sulphur fraction 2	gS/m ³
POS3	Particulate Organic Sulphur fraction 3	gS/m ³
POS4	Particulate Organic Sulphur fraction 4	gS/m ³
POS5	Particulate Organic Sulphur fraction 5	gS/m ³
<i>Dissolved organic matter</i>		
DOC	Dissolved Organic Carbon	gC/m ³
DON	Dissolved Organic Nitrogen	gN/m ³
DOP	Dissolved Organic Phosphorus	gP/m ³
DOS	Dissolved Organic Sulphur	gS/m ³
<i>Electron-acceptors and -donors</i>		
OXY	Dissolved Oxygen	gO ₂ /m ³
SUD	Dissolved sulphide	gS/m ³
CH4	Methane	gC/m ³
FeIIId	Dissolved Iron(III)	gFe/m ³
FeIIpa	Amorphous Iron (oxy)hydroxide	gFe/m ³
FeIIpc	Crystalline Iron (oxy)hydroxide	gFe/m ³
FeIIId	Dissolved Iron(II)	gFe/m ³
FeS	Iron sulphide	gFe/m ³
FeS2	Pyrite	gFe/m ³
FeCO3	Iron carbonate	gFe/m ³

In present D-Water Quality organic matter may consist of maximally six fractions: five particulate fractions (POC1, POC2, POC3, POC4 and POC5) and one dissolved fraction (DOC). For nitrogen, phosphorus and sulphur corresponding fractions exist. Inactive substance POC5 represents the organic matter in stems, branches and large roots of drowned dead terrestrial vegetation. It is only used in conjunction with the drowned vegetation module, fully documented in the Technical Reference Manual, **Detailed description of processes** (Deltares, 2024e).

The mass balances for the dissolved nutrients (NO₃, NH₄, PO₄, Si, TIC) the electron-acceptors (SO₄, SUD and FeIIpa) and detrital organic matter (OM - representing POX) in the water col-

umns are given in the equations below:

$$\frac{\Delta NO_3}{\Delta t} = \text{loads} + \text{transport} + \text{nitrification} - \text{denitrification} - \text{primary production} + \text{atmospheric deposition} \pm \text{sediment exchange flux} \quad (6.23)$$

$$\frac{\Delta NH_4}{\Delta t} = \text{loads} + \text{transport} - \text{nitrification} + \text{mineralization} - \text{primary production} + \text{autolysis} + \text{atmospheric deposition} \pm \text{sediment exchange flux} \quad (6.24)$$

$$\frac{\Delta PO_4}{\Delta t} = \text{loads} + \text{transport} \pm \text{sorption} + \text{mineralization} \pm \text{precipitation/dissolution} + \text{primary production} + \text{autolysis} + \text{atmospheric deposition} \pm \text{sediment exchange flux} \quad (6.25)$$

$$\frac{\Delta Si}{\Delta t} = \text{loads} + \text{transport} + \text{dissolution} - \text{primary production} + \text{autolysis} \pm \text{sediment exchange flux} \quad (6.26)$$

$$\frac{\Delta TIC}{\Delta t} = \text{loads} + \text{transport} + \text{mineralization} - \text{primary production} \pm \text{exchange atmosphere flux} \pm \text{sediment exchange flux} \quad (6.27)$$

$$\frac{\Delta SO_4}{\Delta t} = \text{loads} + \text{transport} + \text{sulphide oxidation} - \text{primary production} - \text{sulphate reduction} \pm \text{sediment return flux} \quad (6.28)$$

$$\frac{\Delta SUD}{\Delta t} = \text{loads} + \text{transport} + \text{sulphate reduction} - \text{sulphide oxidation} \pm \text{sediment return flux} \quad (6.29)$$

$$\frac{\Delta FeIII_{pa}}{\Delta t} = \text{loads} + \text{transport} \pm \text{precipitation-dissolution} - \text{iron reduction} - \text{settling} + \text{resuspension} \quad (6.30)$$

$$\frac{\Delta OM}{\Delta t} = \text{loads} + \text{transport} + \text{mortality} - \text{mineralization} - \text{grazing} - \text{settling} + \text{resuspension} \quad (6.31)$$

Similar mass balances apply to the particulate nutrients (plus settling and resuspension), other iron components (plus oxidation for dissolved iron), methane (minus primary production), and DOX components (minus settling).

Nitrogen is not a conservative substance. Nitrate (NO_3^-) is subjected to denitrification in anaerobic zones of the water system: the sediment and deep water in stratified water systems. This microbial process reduces nitrate into elementary nitrogen, which may escape the water system as nitrogen gas. The opposite process is also possible by means of the fixation of nitrogen into ammonium by blue algae and specific bacteria species. Other processes relevant to nutrient nitrogen are the mineralization of organic nitrogen and the nitrification of ammonium.

Inorganic phosphorus (phosphate) is formed from organic phosphorus during the microbial decomposition of natural organic matter. Other important processes that concern phosphorus are sorption onto (suspended) sediment, its iron containing fraction in particular, and the precipitation of phosphate minerals. The sorption of phosphate is a physical-chemical process,

among other things dependent on the pH. Primary production may raise the pH substantially, which leads to the desorption of phosphate from suspended sediment and the direct availability of this phosphate to primary production. Moreover, phosphate may form vivianite and apatite like minerals. Vivianite is only stable at chemically reducing conditions.

Silicon is only available to phytoplankton in the form of dissolved silicate. The pool of dissolved silicate is gradually replenished by slow dissolution of opal silicate, the residue of the silicate skeletons of diatoms.

Natural detrital organic matter is produced when phytoplankton or other primary producers die. Live and dead organic matter may be consumed by grazers. The resulting particulate and dissolved organic matter in water systems is a continuum of different substances. Fresh natural organic matter is composed of polysaccharides, proteins, lipids, acids and, when originating from diatoms, opal silicate. The various substances contain organic forms of the nutrients nitrogen, phosphorus and sulphur. The production of organic matter (carbon and nutrients) is clarified in [section 6.8](#).

The original components of detritus are partially transformed into highly decomposition resistant (refractory) humic and fulvic substances during the microbial degradation process. Both biochemical and chemical processes are involved. A part of the organic matter remains in a particulate form, a smaller part transforms into dissolved humic and fulvic acids. The bigger part of the organic nutrients are converted into inorganic forms during the decomposition process. However, a smaller part of the nutrients is released at the death of phytoplankton as easily degradable organic substances that are almost instantaneously converted into inorganic species. This process is called autolysis.

The electron-acceptors needed for the decomposition of detrital organic matter include oxygen, nitrate, manganese(IV), iron(III), sulphate and carbon dioxide. In the oxic water column only oxygen is used. The other electron-acceptors are consumed in anoxic water or in the sediment. With the exception of manganese all these electron-acceptors can be modelled with present D-Water Quality. Carbon dioxide and hydrogen are considered implicit in methanogenesis. Oxygen can be simulated stand-alone or combined with any selection of the other electron-acceptors with D-Water Quality.

In view of modelling it is important to be able to relate the model parameters to measured parameters.

- ◇ Kjeldahl-N = ammonium + organic nitrogen
- ◇ Soluble Reactive Phosphorus (SRP) = ortho-phosphate + rapidly desorbing phosphorus (depends on type of filtration prior to chemical analysis and the pH of the water sample)
- ◇ Total phosphorus = ortho-phosphate + organic phosphorus + adsorbed phosphorus + precipitated phosphorus
- ◇ Total nitrogen = nitrate + ammonium + organic nitrogen

Brief descriptions of processes and specific features in D-Water Quality are presented below.

Process	Substances	Comments
Nitrification	NH ₄ NO ₃ (OXY) (Alka)	$NH_4^+ + 2O_2 \rightarrow NO_3^- + 2H^+ + H_2O$ <ul style="list-style-type: none"> ◇ There are two alternative process equations for nitrification. In both alternatives nitrification proceeds proportional to a nitrification rate and to the availability of ammonium and dissolved oxygen. The alternatives differ in their dependency on the ammonium and dissolved oxygen concentration (Michaelis-Menten or linear). ◇ Nitrification can proceed at a (low) background rate, when the temperature decreases below a critically low temperature. Nitrification can proceed at a constant rate when the oxygen concentration is below a critically low level. A constant rate may occur in the water column at zero dissolved oxygen concentration to take into account, that a water column compartment in the model may be depleted from dissolved oxygen on the average, whereas in reality a certain top layer may still contain dissolved oxygen.
Oxygen consumption	OXY	$O_2 + CH_2O \rightarrow CO_2 + H_2O$ <ul style="list-style-type: none"> ◇ The generic approach for oxygen consumption for the degradation of organic matter in both water and sediment considers competition with the consumption of other electron-acceptors such as nitrate, iron, sulphate and carbon dioxide. The oxygen consumption flux is proportional to the mineralization flux. The competition is formulated according to Michaelis-Menten kinetics for limitation.
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Process	Substances	Comments
Denitrification	NO ₃ (OXY) (Alka)	$4NO_3^- + 5CH_2O + 4H^+ \rightarrow 2N_2 + 5CO_2 + 11H_2O$ <ul style="list-style-type: none"> ◇ There are two approaches for denitrification. The simplified approach considers denitrification not coupled to the mineralization flux. ◇ The simplified approach for denitrification in the water column has two alternative process equations for denitrification. In both alternatives denitrification proceeds proportional to a denitrification rate and to the availability of nitrate (Michaelis-Menten or linear). The second option also considers dissolved oxygen concentration as inhibitor. Denitrification can proceed at a low background rate, when the temperature decreases below a critically low temperature. A constant rate may occur in the water column at positive dissolved oxygen concentrations to take into account, that a water column compartment in the model may contain dissolved oxygen on the average, whereas in reality a certain bottom layer may be depleted from oxygen. ◇ In the simplified approach for denitrification in the sediment denitrification is only proportional to the nitrate concentration in the water column. ◇ The generic approach for denitrification in both water and sediment considers competition with the consumption of other electron-acceptors such as oxygen, iron, sulphate and carbon dioxide. The denitrification flux is proportional to the mineralization flux. The competition is formulated according to Michaelis-Menten kinetics for limitation and inhibition.
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Process	Substances	Comments
Iron reduction	SO ₄ FeIIpa (Alka)	$4Fe(OH)_3 + CH_2O \rightarrow 4FeII + CO_2 + 2H_2O + 8OH^-$ <p>◇ The generic approach for iron reduction in both water and sediment considers competition with the consumption of other electron-acceptors such as oxygen, nitrate, sulphate and carbon dioxide. The sulphate reduction flux is proportional to the mineralization flux. The competition is formulated according to Michaelis-Menten kinetics for limitation and inhibition.</p>
Sulphate reduction	SO ₄ SUD	$SO_4^{2-} + 2CH_2O \rightarrow S^{2-} + 2CO_2 + 2H_2O$ <p>◇ The generic approach for sulphate reduction in both water and sediment considers competition with the consumption of other electron-acceptors such as oxygen, nitrate, iron and carbon dioxide. The sulphate reduction flux is proportional to the mineralization flux. The competition is formulated according to Michaelis-Menten kinetics for limitation and inhibition.</p>
Methanogenesis	CH ₄ (POC1-5)	$2CH_2O \rightarrow CO_2 + CH_4$ <p>◇ The generic approach for methanogenesis in both water and sediment considers competition with the consumption of electron-acceptors such as oxygen, nitrate, iron and sulphate. The methanogenesis reduction flux is proportional to the mineralization flux. The competition is formulated according to Michaelis-Menten kinetics for inhibition.</p>
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Process	Substances	Comments
Oxidation	SUD FeIId (OXY) (SO4) (Alka)	<ul style="list-style-type: none"> ◇ The oxidation of total dissolved sulphide, methane and dissolved iron(II) is proportional to their concentrations and the concentration of dissolved oxygen, or in the case of methane also proportional to the concentration of sulphate, or in the case of iron also proportional to the concentration of nitrate.
Iron reduction with sulphides	FeIIpa FeIIpc SUD FeS (Alka)	<ul style="list-style-type: none"> ◇ Both dissolved sulphide and ironsulphide reduce amorphous and crystalline ironoxyhydroxides. All four reduction rates are proportional to the concentrations of both reactants.
Primary production	NH4 NO3 PO4 Si SO4 (TIC) (Phytoplankton) (OXY) (Alka)	<ul style="list-style-type: none"> ◇ Uptake of nutrients takes place as part of primary production. The uptake of nitrogen, phosphorus and silicon is determined by C:N:P:Si ratios which can be different for each type of primary producer. ◇ Ammonium is preferred as the nitrogen nutrient over nitrate.
Atmospheric deposition	NO3 NH4 PO4 SO4	<ul style="list-style-type: none"> ◇ Atmospheric deposition is a zero-order term in $\text{g/m}^2/\text{d}$ (both time and space varying input is possible in D-Water Quality)
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Process	Substances	Comments
Sediment ex- change flux	NO3 NH4 PO4 Si SO4 TIC OXY SUD CH4 FeIII FeII (Alka)	<p>◇ Diffusion of dissolved substances between the water column and the pore water in the sediment. If the concentration in the pore water is higher than in the water column, the substances diffuse to the water column.</p> <p>◇ The diffusional sediment fluxes are produced in different ways for the two approaches for sediment-water interaction. For the simplified S1-S2 approach the return fluxes concern only the nutrients NH4, PO4 and Si. These fluxes are equal to the mineralization fluxes of the organic nutrients. For the layered sediment approach the exchange fluxes result from diffusion. The dissolved concentrations on both sides of the sediment-water interface result from the advection-diffusion-reaction equations (mass balances).</p>
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Process	Substances	Comments
Mineralization	POC1-5 PON1-5 POP1-5 POS1-5 DOC DON DOP DOS NH ₄ PO ₄ SUD TIC (OXY) (NO ₃) (FeIIIpa) (FeIIId) (SO ₄) (CH ₄) (Alka)	<ul style="list-style-type: none"> ◇ Nutrients produced at the mineralization of organic matter are released as dissolved inorganic nutrients. The mineralization of organic nitrogen leads to the release of ammonium only (no nitrate). ◇ The POC2-4 fractions are produced from each other and from POC1 and POC5 (inactive substance for stems and branches of from drowned vegetation). DOC is produced from POC1-4. All substance conversions are proportional to the pertinent mineralization rates. ◇ Optionally, the mineralization rates can be made dependent on the stoichiometry of the organic matter. Organic matter with a low C:N or C:P ratio will have a lower mineralization rate than organic matter with a high C:N or C:P ratio. ◇ Dependent on the difference between actual nutrient stoichiometry of a detritus fraction and the target stoichiometry nutrients will be stripped from that fraction. This implies that the mineralization of N and P proceeds faster than the mineralization of carbon.
Autolysis	NH ₄ PO ₄ Si TIC (Phytoplankton) (OXY) (Alka)	<ul style="list-style-type: none"> ◇ When primary producer die, parts of the nutrients are instantly released to their inorganic dissolved equivalents. ◇ The autolysis fraction is different per primary producer.
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Process	Substances	Comments
Sorption	PO ₄ AAP (IM1-3)	<ul style="list-style-type: none"> ◇ Phosphate is reversibly adsorbed to inorganic matter components IM1-3 (sediment). The adsorption of phosphate may either be only proportional to dissolved phosphate or may saturate according to the adsorption capacity of the sediment. Ad- and desorption may be instantaneous or may slowly proceed towards equilibrium. The sorption rate is proportional to the difference between the actual state and the equilibrium state. ◇ The actual adsorption capacity of sediment is dependent on the pH, the iron content and the presence of dissolved oxygen concentration (the redox potential). Under chemically reducing conditions the adsorption capacity is strongly reduced due to the reduction of phosphate adsorbing iron(oxy)hydroxides.
Precipitation and dissolution phosphate	PO ₄ VIVP APATP	<ul style="list-style-type: none"> ◇ Vivianite P is formed in the absence of dissolved oxygen. The precipitation flux is proportional to the extent of oversaturation of the solution. Vivianite dissolves at the presence of dissolved oxygen. The dissolution flux is proportional to the concentrations of vivianite and dissolved oxygen. ◇ Apatite P forms proportionally to the precipitation of vivianite and the extent of oversaturation of the solution. The dissolution flux is proportional to the concentration of apatite and the extent of undersaturation of the solution.
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Process	Substances	Comments
Precipitation and dissolution electron-acceptors and -donors	SUD SUP FeIIld FeIIlpa FeIIlpc FeIIld FeS FeS2 FeCO3	<ul style="list-style-type: none"> ◇ Sulphide precipitates proportional to the extent of supersaturation of the solution for the free sulphide ion, the concentration of which is derived from an additional process for the pH dependent speciation of sulphide. If iron is modelled SUP should not be modelled, because sulphide precipitation then coincides with iron sulphide precipitation. ◇ Dissolved iron (FeIII or FeII) precipitates or dissolves proportional to the extent of supersaturation or undersaturation. This is formulated as the ratio of a ion activity product and the solubility product minus 1. The ion activity product is calculated from the concentration of the free iron ion that results from an additional process that calculates the speciation of iron in the solution. Additional processes for the speciation of dissolved sulphide and carbonate deliver the concentrations of the cations dependent on the pH. ◇ Crystalline FeIIlpc and pyrite are produced from amorphous FeIIlpa and FeS respectively. The aging of FeIIlpa is proportional to its concentration. The formation of pyrite is proportional to the concentrations of FeS and dissolved hydrogen sulphide.
Dissolution	Si Opal	<ul style="list-style-type: none"> ◇ Opal silicate dissolves in proportion to the extent of undersaturation. The dissolution rate is temperature dependent and proportional to the availability of opal silicate.
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Process	Substances	Comments
Exchange with the atmosphere	OXY TIC CH4	<ul style="list-style-type: none"> ◇ The exchange of oxygen, carbon dioxide and methane between water and atmosphere depends on the extent of super- or undersaturation. The exchange fluxes are functions of the wind speed and flow velocity according the double layer concept. ◇ The carbon dioxide flux depends on the concentration of dissolved carbon dioxide, which is a function of the pH. The carbon dioxide concentration is calculated with an additional process for the carbonate equilibrium. ◇ Methane is also subject to ebullition from the sediment. Any methane produced in excess of saturation of the solution instantly escapes to the atmosphere in bubbles.
Settling ⁶	POC1-4 PON1-4 POP1-4 POS1-4 AAP VIVP APATP OPAL SUP FeIIIpa FeIIIpc FeS FeS2 FeCO3 (DetXS1) (OOXS1)	<ul style="list-style-type: none"> ◇ Settling is proportional to a first order settling velocity (in m/d). ◇ Settling occurs when the actual shear stress is lower than the user-defined critical shear stress for settling. ◇ The actual shear stress is a function of flow velocity and waves. Artificial disturbances such as ships can be added as well. ◇ Each particulate fraction has its own critical shear stress for settling. ◇ In the case of the S1-S2 approach for the modelling of sediment water interaction POX1 settles into DetXS1, POX2-4 settles into OOXs1, AAP into AAPs1, Opal into DetSiS1.
continued on next page		

⁶For a description of the settling and resuspension process refer to [section 6.6](#).

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Process	Substances	Comments
Resuspension	POC1-4 PON1-4 POP1-4 POS1-4 DetCS1-2 DetNS1-2 DetPS1-2 DetSiS1-2 OOCs1-2 OONS1-2 OOPS1-2 OOSiS1-2 AAP VIVP APATP OPAL SUP FeIIIpa FeIIIpc FeS FeS2 FeCO3	<ul style="list-style-type: none"> ◇ Resuspension takes places with a zero-order rate (in g/m²/d) and is proportional to a probability function. ◇ Resuspension takes place when the actual shear stress is higher than the critical shear stress for resuspension. ◇ The sediment layers S1 and S2 each have a critical shear stress for resuspension. The critical shear stress for resuspension is valid for all particulate fractions in the sediment layer. ◇ The resuspension rate of the individual particulate fractions in the sediment layer is proportional to its weight fraction. ◇ In the case of the S1-S2 approach for the modelling of sediment water interaction DetXS1-2 resuspends into POX1, OOXs1-2 into POX2, and DetSiS1-2 and OOSiS1-2 into Opal.
Mortality	POC1-2 PON1-2 POP1-2 POS1-2 POC5 PON5 POP5 POS5 DetCS1-2 DetNS1-2 DetPS1-2 DetSiS1-2 (Phytoplankton) (Vegetation) (microphytobenthos; DiatS1-2)	<ul style="list-style-type: none"> ◇ When phytoplankton or microphytobenthos dies its biomass is turned over into the most rapidly degradable detrital organic matter fractions. The fractionation is different per primary producer. ◇ When drowned vegetation dies its leaf, twig and small roots biomass is turned over into the most rapidly degradable detrital organic matter fractions. The stem, branches and large roots biomass is turned over into fraction POX5.
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Process	Substances	Comments
Grazing	POC1-3 PON1-3 POP1-3 (Primary consumers) (Phytoplankton) (TIC) (OXY) (Alka)	◇ Primary consumers can derive their nutrients from (living or death) organic matter.
pH equilibrium	TIC Alka	◇ The pH can be simulated in a simplified way with process pH_simp. ◇ Buffering by minerals like calcite is not considered, and the process is therefore generally not applicable to the sediment bed. However, the pH can be constrained to avoid incorrect pH.

Remarks:

- ◇ All reaction rates are temperature dependent ([section 6.3](#)).
- ◇ Usually, the sediment is an essential pool of nutrients and organic matter. Refer to [section 6.11](#).
- ◇ Ammonia (NH_3) and nitrite (NO_2^-) are not available as substances in D-Water Quality. Both are already toxic at low concentrations, although concentrations are usually below the toxic levels. In D-Water Quality the ammonia concentration can be derived from the ammonium concentration and the pH.
- ◇ Nutrients can be recycled for an infinite number of times without any losses other than those due to transport, denitrification and burial.

6.7.3 Process equations**Nitrification**

Ammonium is subjected to nitrification. Nitrification is formulated as the sum of a constant background rate (zero-order term) and a concentration dependent rate. The latter depends on dissolved oxygen and ammonium. There are two alternatives for this dependency.

$$R = k_0 + k \times f_{am} \times f_{ox}$$

$$(\text{option 1}) \quad f_{am} = \left(\frac{C_{am}}{K_s + C_{am}} \right) \quad \wedge \quad f_{ox} = \left(\frac{C_{ox}}{K_{sox} + C_{ox}} \right)$$

$$(\text{option 2}) \quad f_{am} = C_{am} \quad \wedge \quad f_{ox} = (1 - f_{ox_{min}}) \times \left(\frac{C_{ox} - C_{oxc}}{C_{oxo} - C_{oxc}} \right)^{10^a} + f_{ox_{min}}$$

with:

$$R \quad \text{rate of nitrification [gN m}^{-3} \text{ d}^{-1}\text{]}$$

k_0	constant background rate [$\text{gN m}^{-3} \text{d}^{-1}$]
k	kinetic constant [$\text{gN m}^{-3} \text{d}^{-1}$]
f_{am}	kinetic factor for ammonium [-] or [gN/m^3]
f_{ox}	kinetic factor for dissolved oxygen [-]
C_{am}	dissolved ammonium concentration [gN m^{-3}]
K_s	half saturation constant [gN m^{-3}]
C_{ox}	dissolved oxygen concentration [$\text{gO}_2 \text{m}^{-3}$]
K_{sox}	half saturation constant for oxygen [$\text{gO}_2 \text{m}^{-3}$]
$f_{ox_{min}}$	minimal value of oxygen limitation function [-]
C_{oxc}	critical dissolved oxygen concentration [gO_2/m^3]
C_{oxo}	optimal dissolved oxygen concentration [gO_2/m^3]
a	curvature coefficient [-]

The constant rate k_0 is made equal to zero when certain criteria with respect to a critically low temperature and a critically high dissolved oxygen concentration are not met.

Oxidation of sulphide

Sulphides oxidizes when oxygen is available. The oxidation rate is the sum of a zero-order background rate and a first-order rate, dependent on the concentrations of both dissolved sulphide and dissolved oxygen:

$$R_{oxi} = k_{0oxi} + k_{oxi} \times C_{sud} \times C_{ox}$$

with:

C_{ox}	dissolved oxygen concentration [$\text{gO}_2 \text{m}^{-3}$]
C_{sud}	dissolved sulphide concentration [gS m^{-3}]
k_{0oxi}	constant background oxidation rate [$\text{gS m}^{-3} \text{d}^{-1}$]
k_{oxi}	oxidation reaction rate [$\text{gO}_2^{-1} \text{m}^3 \text{d}^{-1}$]
R_{oxi}	rate of oxidation [$\text{gS m}^{-3} \text{d}^{-1}$]

Oxidation of iron

Dissolved iron (FeII) oxidizes when oxygen and/or nitrate is available. The oxidation rate is proportional to the concentrations of both dissolved iron and dissolved oxygen or nitrate:

$$R_{oxi} = k_{oxi} \times C_{fed} \times C_{ox}$$

with:

C_{ox}	dissolved oxygen concentration [$\text{gO}_2 \text{m}^{-3}$]
C_{fed}	dissolved iron(II) concentration [gFe m^{-3}]
k_{oxi}	oxidation reaction rate [$\text{gO}_2^{-1} \text{m}^3 \text{d}^{-1}$]
R_{oxi}	rate of oxidation [$\text{gFe m}^{-3} \text{d}^{-1}$]

The oxidation reaction rate may be different for the various dissolved iron species.

Reduction of iron by sulphides

Iron(III)oxyhydroxides are reduced by dissolved sulphide and iron(II)sulphide. The reduction rate is proportional to the concentrations of both reactants:

$$R_{ire} = k_{ire} \times C_{fex} \times C_{sux}$$

with:

C_{fex}	amorphous or crystalline iron(III)oxyhydroxide concentration [gFe m ⁻³]
C_{sux}	dissolved sulphide or iron(II)sulphide concentration [gS or gFe m ⁻³]
k_{ire}	reduction reaction rate [gS ⁻¹ or gFe ⁻¹ m ³ d ⁻¹]
R_{ire}	rate of reduction [gFe m ⁻³ d ⁻¹]

The reduction reaction rates are different for the four reactions.

Oxidation of methane

Methane is oxidized when oxygen or sulphate is available. The two oxidation processes exclude each other. The oxidation rate is the sum of a zero-order background rate and a Michaelis-Menten rate with two limiting substrates:

$$R_{oxi} = k_{0oxi} + k_{oxi} \times \frac{C_{ch4}}{K_s + C_{ch4}} \times \frac{C_{ox}}{K_{sox} + C_{ox}}$$

with:

C_{ch4}	methane concentration [gC m ⁻³]
C_{ox}	dissolved oxygen concentration [gO ₂ m ⁻³]
k_{0oxi}	constant background oxidation rate [gC m ⁻³ d ⁻¹]
k_{oxi}	oxidation reaction rate [gC m ⁻³ d ⁻¹]
R_{oxi}	rate of oxidation [gC m ⁻³ d ⁻¹]

In the formulation for the oxidation with sulphate the concentration of dissolved oxygen is replaced with the concentration of sulphate.

Denitrification, uncoupled

Nitrate is subjected to denitrification. Denitrification is formulated as the sum of a constant background rate (zero-order term) and a concentration dependent rate. The latter depends on dissolved oxygen and nitrate. There are two alternatives for this dependency.

$$R = k_0 + k \times f_{ni} \times f_{ox}$$

(option 1) $f_{ni} = \left(\frac{C_{ni}}{K_s + C_{ni}} \right) \quad \wedge \quad f_{ox} = 1.0 - \left(\frac{C_{ox}}{K_{sox} + C_{ox}} \right)$

(option 2) $f_{ni} = C_{ni} \quad \wedge \quad f_{ox} = \left(\frac{C_{oxc} - C_{ox}}{C_{oxc} - C_{oxo}} \right)$

with:

R	rate of denitrification [gN m ⁻³ d ⁻¹]
k_0	constant background rate [gN m ⁻³ d ⁻¹]
k	kinetic constant [gN m ⁻³ d ⁻¹]
f_{ni}	kinetic factor for ammonium [-] or [gN/m ³]
f_{ox}	kinetic factor for dissolved oxygen [-]
C_{ni}	dissolved ammonium concentration [gN m ⁻³]
K_s	half saturation constant [gN m ⁻³]
C_{ox}	dissolved oxygen concentration [gO ₂ m ⁻³]
K_{sox}	half saturation constant for oxygen [gO ₂ m ⁻³]
f_{oxmin}	minimal value of oxygen limitation function [-]
C_{oxc}	critical dissolved oxygen concentration [gO ₂ /m ³]
C_{oxo}	optimal dissolved oxygen concentration [gO ₂ /m ³]

The constant rate k_0 is made equal to zero when certain criteria with respect to a critically low temperature and a critically high dissolved oxygen concentration are not met. Note that

the above formulations imply that denitrification is not coupled to the decomposition of detrital organic matter.

Sorption of phosphate

Three options are available for the formulation of the sorption of rapidly desorbing phosphate (AAP). The simplest formulation (option 0) is based on the assumption that the concentration of adsorbed phosphate is linearly proportional to the concentration of dissolved phosphate according to a constant distribution coefficient. The equilibrium is reached instantaneously.

Both other options take the Langmuir model for adsorption and the adsorption capacity of suspended sediment as starting points. Option 1 ignores the pH, temperature and redox potential dependencies, whereas option 2 takes these into account. The essence of the formulations can be described with:

$$K_{ads} = \frac{C_{pha} \times OH^a}{C_{phd} \times C_{ads}}$$

$$C_{adst} = f_{cor} \times \sum_{i=1}^3 (f_{Fe_i} \times C_{im_i}) \times \frac{1}{56 \times 10^3 \times \varphi}$$

$$R_{sorp} = k_{sorp} \times (C_{phae} - C_{pha}')$$

with:

a	stoichiometric reaction constant, equal to 0 for option 1 [-]
C_{ads}	free adsorbent concentration [mol Fe l _w ⁻¹]
C_{adst}	total molar concentration of adsorption sites [mol Fe l _w ⁻¹]
C_{im_i}	concentration of inorganic matter fractions $i = 1, 2, 3$ [gDW m _ℓ ⁻³]
C_{pha}	adsorbed phosphate concentration [moleP l _w ⁻¹]
C_{pha}'	adsorbed phosphate concentration after the previous time-step [gP m _ℓ ⁻³]
C_{phae}	equilibrium adsorbed phosphate concentration [mol P l _w ⁻¹]
C_{phd}	dissolved phosphate concentration [mol P l _w ⁻¹]
f_{cor}	correction factor for oxidised iron (III) fraction, equal to 1 for option 1 [-]
f_{Fe_i}	fraction reactive iron (III) in inorganic matter fractions $i = 1, 2, 3$ [gFe gDW ⁻¹]
k_{sorp}	sorption reaction rate [d ⁻¹]
K_{ads}	adsorption equilibrium constant [mol ^{a-1} l _w ^{a-1}]
OH	adsorption equilibrium constant [mol l _w ⁻¹]
R_{sorp}	rate of adsorption or desorption [gP m _ℓ ⁻³ d ⁻¹]
φ	porosity [-]

With f_{cor} the effect on the adsorption capacity of the redox potential represented by the presence or the absence of dissolved oxygen can be taken into account.

The sorption process can be simulated as a near equilibrium process by assigning high value to the adsorption and desorption rates k_{sorp} . The equilibrium adsorbed phosphate concentration C_{phae} can be calculated. The adsorption equilibrium constant K_{ads} is temperature dependent for option 2.

Precipitation and dissolution of vivianite and apatite

The precipitation of vivianite and apatite is formulated with first-order kinetics. The difference between the actual dissolved phosphate concentration and the equilibrium dissolved concentration is the driving force. Precipitation of vivianite can not proceed when the dissolved oxygen concentration is above a critical value. The precipitation rate of apatite is propor-

tional to the rate of vivianite. The dissolution of vivianite depends on the dissolved oxygen concentration. The formulations are as follows:

$$\begin{aligned} R_{prc_1} &= k_{prc_1} \times (C_{phd} - C_{phde_1}) \\ R_{sol_1} &= k_{sol_1} \times C_{phpr_1} \times C_{ox} \\ R_{prc_2} &= k_{prc_2} \times (C_{phd} - C_{phde_2}) \\ R_{sol_2} &= k_{sol_2} \times C_{phpr_2} \times (C_{phde} - C_{phd}) \end{aligned}$$

with:

C_{ox}	dissolved oxygen concentration [gO ₂ m ⁻³]
C_{phd}	dissolved phosphate concentration [gP m ⁻³]
C_{phde}	equilibrium dissolved phosphate concentration [gP m ⁻³]
C_{phpr}	precipitated phosphate concentration [gP m ⁻³]
k_{prc}	precipitation reaction rate [d ⁻¹]
k_{sol}	dissolution reaction rate [m ³ w gO ₂ ⁻¹ d ⁻¹]
R_{prc}	rate of precipitation [gP m ⁻³ d ⁻¹]
R_{sol}	rate of dissolution [gP m ⁻³ d ⁻¹]
<i>subscript</i>	1 indicates vivianite, 2 indicates apatite

Dissolution of opal silicate

Opal silicate (OPAL) dissolves slowly according to the following (pseudo) second-order kinetics:

$$R_{sol} = k_{sol} \times C_{sip} \times \left(C_{side} - \frac{C_{sid}}{\varphi} \right)$$

with:

C_{sid}	dissolved silicate concentration [gSi m ⁻³]
C_{side}	equilibrium dissolved silicate concentration [gSi m ⁻³]
C_{sip}	opal silicate concentration [gSi m ⁻³]
k_{sol}	(pseudo) second-order kinetic constant [m ³ gSi ⁻¹ d ⁻¹]
R_{sol}	rate of opal silicate dissolution [gSi m ⁻³ d ⁻¹]
φ	porosity [-]

Precipitation and dissolution of iron and sulphur

Dissolved iron (FeIII or FeII) precipitates or dissolves proportional to the extent of supersaturation or undersaturation. This is formulated as follows:

$$\begin{aligned} R_{prc} &= k_{prc} \times \left(\frac{IAP}{SOL} - 1 \right) \\ R_{dis} &= k_{dis} \times C_{FeX} \times \left(1 - \frac{IAP}{SOL} \right) \end{aligned}$$

with:

C_{FeX}	concentration of iron mineral X [gFe m ⁻³]
IAP	ion activity product [mol L ⁻¹]
SOL	solubility product [mol L ⁻¹]
k_{prc}	precipitation reaction rate [gFe m ⁻³ d ⁻¹]
k_{dis}	dissolution reaction rate [d ⁻¹]
R_{dis}	rate of dissolution [gFe m ⁻³ d ⁻¹]

R_{prc} rate of precipitation [$\text{gFe m}^{-3} \text{d}^{-1}$]

The ion activity product is calculated from the concentration of the free iron ion that results from an additional process that calculates the speciation of iron in the solution. Additional processes for the speciation of dissolved sulphide and carbonate deliver the concentrations of the cations dependent on the pH.

The aging of FeIIIpa into FeIIIpc follows from:

$$Ra = ka \times C_{Fea}$$

with:

C_{Fea} concentration of amorphous FeIIIpa [gFe m^{-3}]
 ka aging reaction rate [d^{-1}]
 Ra rate of aging [$\text{gFe m}^{-3} \text{d}^{-1}$]

The formation of pyrite follows from:

$$Ra = ka \times C_{FeS} \times H_2S$$

with:

C_{FeS} concentration of FeS [gFe m^{-3}]
 H_2S concentration of H_2S [gS m^{-3}]
 k_{pyr} formation of FeS_2 [$\text{gS}^{-1} \text{m}^3 \text{d}^{-1}$]
 R_{pyr} rate of pyrite formation [$\text{gFe m}^{-3} \text{d}^{-1}$]

If iron is modelled, substance particulate sulphide (SUP) should not be modelled, because sulphide precipitation then coincides with iron sulphide precipitation. If iron is not modelled the precipitation and dissolution of SUP is proportional to the extent of supersaturation for the free sulphide ion as follows from:

$$R_{prc} = 32\,000 \times k_{prc} \times (C_s - C_{se})$$

$$R_{dis} = 32\,000 \times k_{dis} \times (C_{se} - C_s)$$

with:

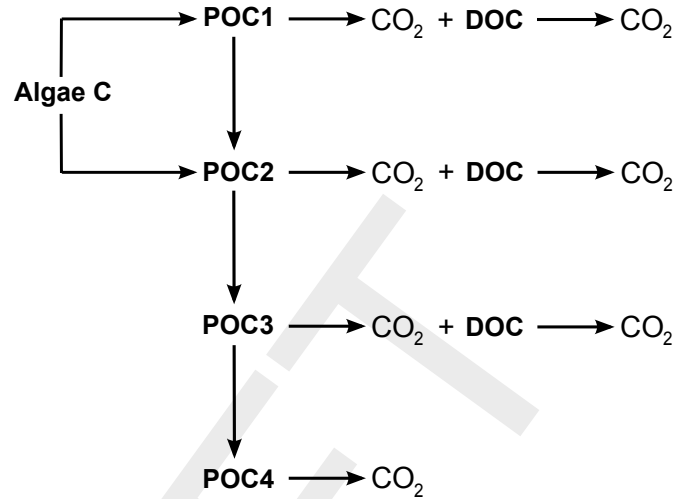
C_s concentration of the free sulphide ion [mole L^{-1}]
 C_{se} equilibrium concentration of the free sulphide ion [mole L^{-1}]
 k_{prc} precipitation reaction rate [d^{-1}]
 k_{dis} dissolution reaction rate [d^{-1}]
 R_{prc} rate of precipitation [$\text{gS m}^{-3} \text{d}^{-1}$]
 R_{dis} rate of dissolution [$\text{gS m}^{-3} \text{d}^{-1}$]

The concentrations of the sulphide ion are derived from an additional process for the pH dependent speciation of sulphide.

Decomposition of organic matter (POC1-5/DOC)

The decomposition of detrital organic matter is described as the serial mineralization and conversion of six fractions. Each mineralization flux has a proportional conversion flux. The fractions are produced, converted and mineralized according to the following scheme (bold parameters are actually simulated):

POC1 is the fast decomposing detritus fraction, POC2 the medium slow decomposing fraction, POC3 the slow decomposing fraction, and POC4 the particulate refractory fraction. DOC



represents dissolved refractory organic matter. POC5 contains the organic matter in stems, branches and roots of dead vegetation that may be subjected to (very) slow decomposition. POC5 is not transported in the model. CO₂ is modelled as TIC (total inorganic carbon). The scheme represents carbon, but is similarly applicable to nitrogen, phosphorus and sulphur.

The mineralization rate is a function of limiting factors related to the electron acceptor used, the preferential stripping of nutrients, and the nutrient availability for bacteria. Mineralization has been formulated as the following first-order kinetic process:

$$R_{min} = f_{el} \times f_{acc} \times k_{min} \times Cx$$

$$k_{min} = k_{min_{min}} + f_{nut} \times (k_{min_{max}} - k_{min_{min}})$$

with:

Cx	organic carbon, nitrogen or phosphorus concentration [gC/N/P m ⁻³]
f_{acc}	acceleration factor for nutrient stripping [-]
f_{el}	limiting factor for electron acceptors [-]
f_{nut}	limiting factor for nutrient availability [-]
k_{min}	first-order mineralization rate [d ⁻¹]
max	index for the maximal value, the upper limit
min	index for the minimal value, the lower limit

Consumption of electron-acceptors and methanogenesis

The consumption of the electron-acceptors is coupled to the mineralization of organic matter. The relative contributions of the electron-acceptors oxygen (OXY), nitrate (NO₃; denitrification), iron (FeIIIpa; iron reduction), sulphate (SO₄; sulphate reduction) and carbon dioxide depend on Michaelis-Menten kinetics for limitation and inhibition. The consumption of carbon dioxide and hydrogen is implicit in the production of methane (CH₄; methanogenesis), so that in the model methane is directly produced from organic carbon. The formulations are as follows:

$$fli_i = \frac{Ce_i}{Ksl_i + Ce_i} \times \left(1.0 - \frac{Ce_{i-1}}{Ksi_{i-1} + Ce_{i-1}}\right)$$

$$frli_i = \frac{fli_i}{\sum_{i=1}^n fli_i}$$

$$Rcns_i = a_i \times frli_i \times Rtmin$$

with:

a_i	stoichiometric constant of limiting electron-acceptor i [gEA/gC]
Ce_i	concentration of limiting electron-acceptor i [gEA m ⁻³]
Ce_{i-1}	concentration of inhibiting electron-acceptor $i - 1$ [gEA m ⁻³]
fli_i	limitation-inhibition function for electron-acceptor i or methane [-]
$frli_i$	fraction of organic matter mineralization connected with the consumption of electron-acceptor i or the production of methane [-]
Ksl_i	half-saturation concentration of limiting electron-acceptor i [gEA m ⁻³]
Ksi_{i-1}	half-saturation concentration of inhibiting electron-acceptor $i - 1$ [gEA m ⁻³]
$Rcns_i$	consumption rate of electron-acceptor i [gEA m ⁻³ day ⁻¹] or production rate of methane [gC m ⁻³ day ⁻¹]
$Rtmin$	total mineralization rate of organic matter [gC m ⁻³ day ⁻¹]

The reduction of oxygen is only subjected to a limitation function, methanogenesis only to an inhibition function. Denitrification is inhibited by oxygen, sulphate and iron reduction by nitrate, and methanogenesis by sulphate. This approach allows the overlap of all reduction processes in each water or sediment layer. Iron and sulphate are ignored in the formulations when they are not modelled.

Exchange with the atmosphere

Similar formulations apply to the exchange of oxygen, carbon dioxide and methane between water and atmosphere as based on the double layer concept with transfer coefficients. The exchange of oxygen with the atmosphere (reaeration) is discussed in (section 6.5.3).

Additionally, methane ebullition is included in the Processes Library. The rate of this process is proportional to the quantity of methane produced, when the dissolved methane concentration exceeds the pressure and temperature dependent saturation concentration.

6.8 Primary producers: phytoplankton

6.8.1 Concepts

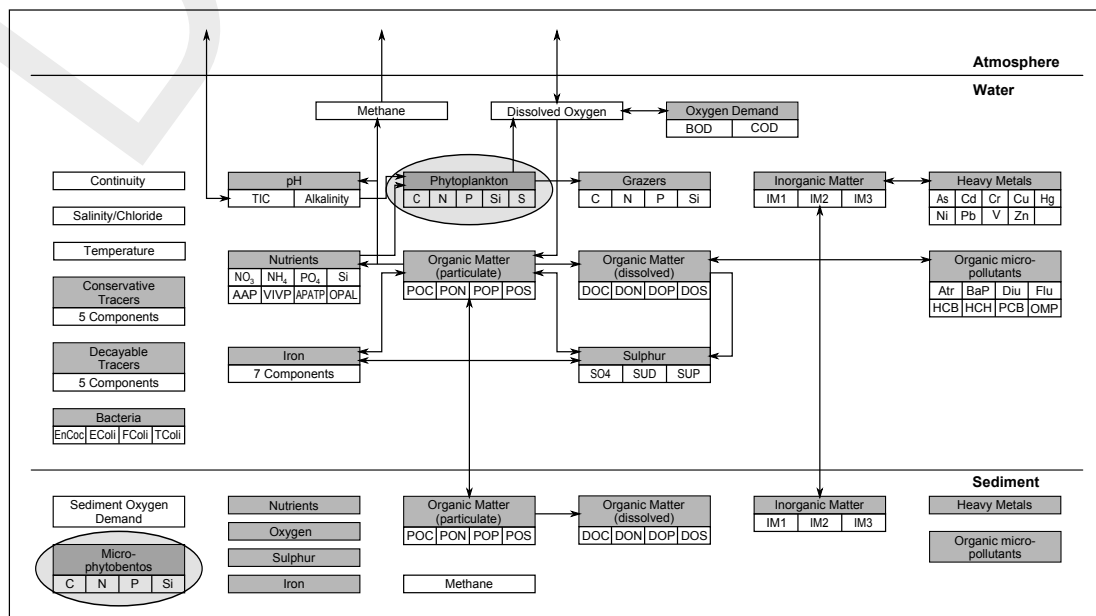


Figure 6.7: Overview of substances. Primary producers: phytoplankton

What is primary production?

All organisms require some form of energy for maintenance, growth and reproduction. Basically there are two sources of energy that are widely used:

- 1 Light (solar energy) is directly used by so-called primary producers,
- 2 Organic material resulting from primary production is utilised directly or indirectly by consumers via the food web.

Therefore, it is fair to say that life on earth as we know it would be impossible without primary production. Primary production occurs both in aquatic and in terrestrial environments. Although there is a great diversity among primary producers, the basic process is very similar:

Light + Water + Carbon dioxide → Sugar + Oxygen

The most important primary producers in the aquatic environment are:

- ◇ Algae, which include relatively large, plant-like organisms (weeds) and planktonic forms.
- ◇ Cyano-bacteria (often referred to as blue green algae).
- ◇ Microphytobenthos (mostly benthic diatoms).
- ◇ Submerged and emerging macrophytes (vascular water plants).

In terms of the total amount of energy that is fixed, planktonic algae and cyano-bacteria are the most important primary producers.

Environmental requirements

Biologically speaking, phytoplankters are relatively primitive plantlike organisms. They require considerable amounts of nutrients and solar energy. In theory both of these factors could become limiting, but the question is where and when. Also the physiological data indicate that species of phytoplankton differ greatly in nutrient requirements, efficiency of solar energy fixation (photosynthesis) and (potential) net growth rates.

The sun provides the energy, at a rate per square metre of surface area that depends upon latitude, season, time of day and cloud cover. The energy must be shared among all the phytoplankton cells floating in the water column below that square metre of surface area, with an allowance set aside for reflection from the water surface and absorption by the bulk water and its contents other than phytoplankton. The absorption (extinction) of light depends on the concentrations of absorbing substances such as algae biomass, detrital organic matter, inorganic sediment and water. The extinction of water with dissolved (inorganic) substances is indicated as the background extinction. The more phytoplankton there is, the less solar energy is available for each, until the energy per phytoplankton cell is too small to sustain growth. At that point, solar energy becomes limiting to the phytoplankton biomass.

Plants also require about a dozen chemical elements for a normal development, among which are nitrogen, phosphorus, sulphur, calcium, potassium, magnesium and iron. The requirements for each element vary widely. Three macro-nutrients, which are often reported as limiting factors (nitrogen, phosphorus, and silicon), are generally considered to be potential biomass limiting factors for phytoplankton, along with solar energy.

Nitrogen and phosphorus are vital to all phytoplankton species. Nitrogen is an essential component of cell proteins such as enzymes, for genetic material, and of light-sensitive pigments like chlorophyll-a, which are used for fixation of solar energy. Because of its importance to many vital physiological processes, nitrogen deficiencies cannot be tolerated for long. In

aquatic systems nitrogen is available as ammonium and nitrate. Nitrogen gas (N₂) can only be used by nitrogen fixating algae.

Phosphorus is an important component of proteins, nucleic acids, and lipids (e.g., in the cell walls). Coupling and uncoupling of ortho-phosphate groups to certain sugars are the main reactions by which energy is stored or released in the cell. Phytoplankton cells are usually less sensitive to phosphorus than to nitrogen deficiencies, hence survival at extremely low internal phosphorus concentrations is often possible for some time.

Silicon is essential to only one phytoplankton group, diatoms. These species use silicon to build strong skeletons surrounding the cell walls.

Eutrophication

Humans are special among the consumers since man's activities have strongly affected the environmental conditions on earth particularly during the the last two centuries. Since then the amounts of various substances, which are released into the environment, have increased dramatically. Many of these are seriously toxic, but other chemicals are on the contrary beneficial to certain organisms. Among these are several compounds of the elements nitrogen and phosphorus which are required by species of phytoplankton, among others.

As a result the concentrations of these plants have increased up to a level where they are considered a nuisance in many waters. This process, which is called eutrophication, is accompanied by several objectionable symptoms: it gives the water a green, turbid appearance; it can cause bad odours; it may harm other organism because the minimum daily oxygen level can become extremely low during the night due to phytoplankton respiration; it can even cause the water to become completely deprived of oxygen (anaerobic) when a bloom declines rapidly, since the biological degradation processes consume large amounts of oxygen; it may cause clogging of filters in drinking water purification systems. Some species of phytoplankton such as cyano bacteria or dinoflagellates may also induce toxic effects in primary or secondary consumers.

6.8.2 Modelling framework

The substances that can be modelled in D-Water Quality in relation to phytoplankton and microphytobenthos are:

Name of D-Water Quality substance	Description	Unit
<i>Phytoplankton: DYNAMO</i>		
Diat	Diatoms	gC/m ³
Green	Non-diatoms	gC/m ³
<i>Phytoplankton: BLOOM</i>		
FDIATOMS	Freshwater diatoms (E- and N-phenotype)	gC/m ³
FFLAGELA	Freshwater flagellates (E-phenotype)	gC/m ³
GREENS	Green algae (E-, N- and P-phenotype)	gC/m ³
APHANIZO	Aphanizomenon (E-, N- and P-phenotype)	gC/m ³

Name of D-Water Quality substance	Description	Unit
APHANFIX	Nitrogen-fixing Aphanizomenon (E-, N- and P-phenotype)	gC/m ³
MICROCYS	Microcystis (E-, N- and P-phenotype)	gC/m ³
OSCILAT	Oscillatoria (E-, N- and P-phenotype)	gC/m ³
BLUEGRN	Blue green algae (E-, N- and P-phenotype)	gC/m ³
MDIATOMS	Marine diatoms (E-, N- and P-phenotype)	gC/m ³
MFLAGELA	Marine flagellates (E-, N- and P-phenotype)	gC/m ³
DINOFLAG	Dinoflagellates (E-, N- and P-phenotype)	gC/m ³
DINOMIX	Mixotrophic dinoflagellates (E-, N- and P-phenotype)	gC/m ³
PHAEOCYS	Phaeocystis (E-, N- and P-phenotype)	gC/m ³
ULVAS	Suspended Ulva (E-, N- and P-phenotype)	gC/m ³
ULVAF	Rooted Ulva (E-, N- and P-phenotype)	gC
<i>Microphytobenthos: DYNAMO</i>		
DiatS1	Benthic diatoms in layer S1	gC/m ²
DiatS2	Benthic diatoms in layer S2	gC/m ²

Two modules are available for the modelling of phytoplankton, BLOOM and DYNAMO. These modules are alternatives, that differ strongly with respect to ruling concepts, process formulations and process details. They can not be used simultaneously. However, the modules share processes with respect to light extinction, settling and resuspension. Both modules include the same major processes: the production and mortality of algae biomass, the uptake and excretion of the nutrients and the production and consumption of dissolved oxygen and carbon dioxide. The modelling of all other processes to which the nutrients are subjected and the modelling of detrital organic matter partially produced from biomass are described in [section 6.7](#). [section 6.5](#) provides the description of the modelling of other processes for dissolved oxygen. BLOOM is also capable of the simulation of Ulva like macro algae that can attach themselves to the sediment. DYNAMO allows for the modelling of microphytobenthos by means of an additional process for primary production and mortality in the sediment, when this is modelling according to the S1-S2 approach.

DYNAMO versus BLOOM

BLOOM is a multi-species algae model, based on an optimisation technique that distributes the available resources in terms of nutrients and light among the algae species ([WL | Delft Hydraulics, 1991a, 1992](#); [Los and Brinkman, 1988](#)). BLOOM optimises the species composition to obtain the overall maximum growth rate under the given conditions. A large number of groups and/or species of algae and even different phenotypes within one species can be considered. BLOOM distinguishes between three phenotypes: under nitrogen limiting conditions, under phosphorus limiting conditions and under light limiting conditions. Algae living in the water column (phytoplankton) and (macro)algae on the sediment can be included with their specific ecophysiological characteristics (this has been implemented for *Ulva*). A database for

15 algae groups and species is part of D-Water Quality.

DYNAMO is based on a more traditional model of primary production using Monod-kinetics for the calculation of growth rates (WL | Delft Hydraulics, 1989). Two groups of algae are considered: diatoms and all non-diatoms (referred to as 'Green' algae). The main difference between the types is that diatoms utilise silica as an essential nutrient, while 'non-diatoms' do not.

The selection of the appropriate algae module will often depend on the modelling objective. However, the availability of data (field observations and model coefficients), model status and possibly the amount of required computation time can be important too.

DYNAMO is recommended for general reconnaissance studies, in which distinction of different species and competition between species are not considered of prime importance. Using DYNAMO the aim should be to calculate overall primary production in terms of the total algal biomass. DYNAMO may also be selected for eutrophication pre-studies focussing on nutrient mass balances and the primary effects of the decrease or increase of the nutrient loads.

BLOOM should be selected for phytoplankton simulations, when the prediction of specific algae species and their biomass in a setting of multi-species competition is the primary goal of the application. BLOOM will include the inter-species competition for resources (light, nutrients). Using BLOOM can for example be of importance, if nuisance algae such as blue green algae species need to be included in the model.

Before making a choice, you should preferably have a detailed picture of the variables that need to be simulated and the significance of the quality of the calculations. First of all, both models can simulate algal growth rates and resulting biomass concentrations. To give a simplified picture of the outcome of these calculations, the DYNAMO approach will generally give a more linear picture of biomass development, while the BLOOM approach can simulate non-linear, more dynamic behaviour as well.

In general, the availability and accuracy of the data needed to determine the values of the model coefficients as well as the data for model validation limit the reliability of modelling results. Naturally, this is true for algae modelling as well. Since the DYNAMO approach requires less coefficients, you might be tempted to assume that a scarce data base will automatically point to the use of DYNAMO. You should note however, that describing complex processes by simple equations makes it necessary to tune the coefficients for local conditions. Moreover, DYNAMO-coefficients may be rather hard to determine and the modelling results can be very sensitive to the values of these coefficients. It is therefore recommended to carefully inspect the available data before choosing a modelling approach.

Furthermore, it can be wise to investigate whether one of the models has already been validated for a system that is similar to the system that should be modelled. If so, choosing the model that has proven successful under those conditions can be particularly helpful if the available data set is limited. Validation of the model results for a wide range of both freshwater and marine systems has resulted in a data base with coefficients for 13 algal groups and species for which calibration is hardly required. Obviously, this is a special advantage of BLOOM.

Mass balance

The general mass balance for phytoplankton (in the water column) is given in the equation below for both DYNAMO and BLOOM:

$$\frac{\Delta \text{Phytoplankton}}{\Delta t} = \text{loads} + \text{transport} - \text{settling} + \text{resuspension} + \text{gross primary production} - \text{respiration} - \text{mortality} \quad (6.32)$$

Phytoplankton produces oxygen in quantities relative to the gross production of organic matter. The algae consume dissolved oxygen for respiration.

Dead phytoplankton biomass is converted to the inorganic nutrients (autolysis) and the detritus pool in the water column (see [section 6.7](#)). Settled algae biomass only dies in the sediment, either instantly in the case of the S1-S2 approach, or slowly when sediment-water interaction is modelled according to the layered sediment approach. The dead biomass is converted to the sediment detritus pools. Resuspended benthic algae biomass is turned over instantly in to the detritus pools in the water column.

Grazing is added to the mass balance for algae biomass when one of the available grazing modules of D-Water Quality is included in a model.

Brief description and relevant notes of processes:

Process	Substances	Comments
Gross primary production	All phytoplankton (NH ₄) (NO ₃) (PO ₄) (Si) (OXY) (TIC) (Alka) (SO ₄)	<ul style="list-style-type: none"> ◇ Gross primary production is proportional to the biomass concentration and a gross primary production (growth) rate. ◇ Algae consume inorganic nutrients and produce dissolved oxygen proportional to net primary production. Only diatoms consume silicon as a nutrient. The uptake of nitrogen, phosphorus and silicon is determined by C:N:P:Si ratios which can be different for each type of primary producer. ◇ The chlorophyll content of algae is species specific. The total chlorophyll-a concentration is equal to the sum of the contributions of all algae species. ◇ (Major) Limiting factors are light availability and nutrient availability. BLOOM and DYNAMO have different formulations. ◇ The inclusion of TIC and/or SO₄ in a model is optional for BLOOM. DYNAMO ignores sulphur components.
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Process	Substances	Comments
Respiration	All phytoplankton (NH4) (PO4) (Si) (OXY) (TIC) (Alka) (SUD)	<ul style="list-style-type: none"> ◇ Respiration is the sum of growth respiration and maintenance respiration. Growth respiration is a species specific fraction of gross production, included in the growth rate for BLOOM. Maintenance respiration is proportional to the algal biomass and a respiration rate.
Mortality and autolysis	All phytoplankton POX1-2 (Opal) (NH4) (PO4) (Si) (OXY) (TIC) (Alka) (SUD)	<ul style="list-style-type: none"> ◇ Algal mortality is proportional to the biomass concentration and an overall mortality rate. ◇ Note that grazing as an additional loss process is only considered when one of the grazing modules is included in the model. Otherwise, the loss due to grazing should be incorporated in the mortality rate. ◇ Next to temperature dependent mortality, mortality caused by salinity stress can also be included. The mortality rate is a combined function of the temperature and the chloride concentration. Freshwater algae start dying when salinity increases. Marine algae start dying when salinity drops. ◇ The simulation of POS1-2 and SUD is optional for BLOOM.
Settling ⁷	All phytoplankton (POX1-2) (Opal) DetXS1	<ul style="list-style-type: none"> ◇ Settling only takes place when the bottom shear stress drops below a critical value. Settling thus depends on the flow velocity and turbulence in the water. ◇ Settling is proportional to the biomass concentration and a species specific settling velocity. ◇ Algae biomass settles in DetXS1 in case of the S1-S2 approach for the sediment.
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⁷For a detailed description of the settling and resuspension process refer to [section 6.6](#).

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Process	Substances	Comments
Resuspension ¹¹	DiatS1 DiatS2 BLOOM algae (POX1-2)	<ul style="list-style-type: none"> ◇ Resuspension takes place with a zero-order rate (in g/m²/d) and is proportional to a probability function. ◇ Resuspension takes place when the actual shear stress is higher than the critical shear stress for resuspension. ◇ The sediment layers S1 and S2 each have a critical shear stress for resuspension. The critical shear stress for resuspension is valid for all particulate fractions in the sediment layer. ◇ The resuspension rate of the individual particulate fractions in the sediment layer is proportional to its weight fraction.
Grazing ⁸	All phytoplankton (Primary consumers) (POX1-3) (Opal) (OXY) (TIC) (Alka)	<ul style="list-style-type: none"> ◇ Primary consumers can derive their nutrients from living and detrital organic matter. ◇ Taking grazing into account requires the inclusion of a grazing module in a model.

Remarks:

- ◇ The total light extinction in the water column is the sum of background extinction (water itself and non-modelled substances) and extinction due to phytoplankton, detritus and inorganic matter.
- ◇ Process rates are temperature dependent as indicated in [section 6.3](#) ($k = k_r \times kt^{(T-T_r)}$). However, it is important to note that DYNAMO has a reference temperature of 20 °C, whereas BLOOM has a reference temperature of 0 °C.

6.8.3 Process equations**Phytoplankton: BLOOM**

BLOOM distinguishes species groups like marine diatoms and dinoflagellates. Within a species group up to three phenotypes can be distinguished: the N-limited phenotype, the P-limited and the E-limited phenotype. The phenotypes occur under respectively nitrogen limiting conditions, phosphorus limiting conditions and light (energy) limiting conditions. Phenotypes have distinct growth rates, mortality rates, nutrient-carbon ratios, etc.

The primary production for BLOOM is simulated with an optimisation technique (LP). This technique delivers the biomass for each (included) algae phenotype at the end of a time step by means of solving a set of linear equations and inequalities (constraints), thereby maximising the total net primary production. The principles of the constraints are as follows:

⁸For a detailed description of grazing refer to [section 6.9](#).

for nutrients,

$$Ctnut_k = Cnut_k + \sum_{i=1}^n (anut_{k,i} \times Calg_i) - Cnutc_k$$

for energy (light),

$$eca = \sum_{i=1}^n (ec_i \times Calg_i)$$

$$ecmin_i \leq eca \leq ectmax_i$$

$$ecmin_i = ectmin_i - ecb$$

$$ectmax_i = ectmax_i - ecb$$

$$Ia_i = \frac{I_{top} \times (1 - e^{-ectmax_i \times Ha})}{ectmax_i \times Ha}$$

$$Ia_i = f(Efc_i)$$

for growth,

$$Calg2_i \leq Calg1_i \times e^{((kgp_i \times Ef_i - krsp_i) \times Dtb)}$$

for mortality,

$$Calg2_i = Calg1_i \times e^{(-kmrt_i \times Dtb)}$$

with:

<i>anut</i>	stoichiometric constant of nutrient k originating from dissolved inorganic nutrient over organic carbon in algae biomass [gN/P/Si gC ⁻¹]
<i>Calg</i>	algae biomass concentration [gC m ⁻³]
<i>Calg1</i>	biomass of algae species <i>j</i> at time <i>t</i> ₁ [gC m ⁻³]
<i>Calg2</i>	biomass of algae species <i>j</i> at time <i>t</i> ₂ [gC m ⁻³]
<i>Cnut</i>	concentration of dissolved inorganic nutrient k [gN/P/Si m ⁻³]
<i>Cnutc</i>	threshold concentration of dissolved inorganic nutrient <i>k</i> [gN/P/Si m ⁻³]
<i>Ctnut</i>	concentration of total available nutrient <i>k</i> [gN/P/Si m ⁻³]
<i>ec</i>	specific extinction coefficient of an algae species type [m ² gC ⁻¹]
<i>eca</i>	total extinction coefficient of all algae [m ⁻¹]
<i>ect</i>	total extinction coefficient [m ⁻¹]
<i>ecmin</i>	minimum extinction coefficient of algae due to background extinction [m ⁻¹]
<i>ectmin</i>	minimum total extinction coefficient due to background extinction [m ⁻¹]
<i>ectmax</i>	maximum extinction coefficient of algae needed to avoid self shading [m ⁻¹]
<i>ectmax</i>	maximum total extinction coefficient to avoid self shading of algae <i>i</i> [m ⁻¹]
<i>Ef</i>	light efficiency factor [-]
<i>Efc</i>	critical light efficiency factor [-]
<i>Ha</i>	time step average depth of a water compartment or water layer [m]
<i>Ia</i>	critical depth average light intensity [W m ⁻²]
<i>Itop</i>	light intensity at the top of a water compartment/layer [W m ⁻²]
<i>kgp</i>	potential specific gross primary production rate of the E-phenotype of an algae species [d ⁻¹]
<i>kmrt</i>	specific mortality rate of an algae species type [d ⁻¹]
<i>krsp</i>	specific maintenance respiration rate of the E-phenotype of an algae species [d ⁻¹]
<i>z</i>	depth [m]

Δt	time step [d]
i	index for algae species type [-]
k	index for nutrients, 1 = nitrogen, 2 = phosphorus, 3 = silicon [-]
n	number of algae species types, maximum allowed is 15 [-]

The optimisation technique finds the new biomass of each algal phenotype at the end of a time step. The rates of growth, production, mortality and autolysis are derived from the change of the algae biomasses over a time step.

$$Rgr_i = \frac{(Calg2_i - Calg1_i)}{Dt}$$

$$Rgp_i = Rgr_i + Rrsp_i + Rmrt_i$$

$$Rnp_i = Rgp_i - Rrsp_i$$

$$Rmrt_i = \frac{kmrt_i \times (Calg2_i + Calg1_i)}{2}$$

$$Raut_i = f_{aut_i} \times Rmrt_i$$

with:

f_{aut}	fraction of dead algae biomass autolysed [-]
$Raut$	autolysis rate for dead algae biomass [gC m ⁻³ d ⁻¹]
Rgp	gross primary production rate [gC m ⁻³ d ⁻¹]
Rgr	growth rate for organic carbon [gC m ⁻³ d ⁻¹]
$Rmrt$	mortality rate [gC m ⁻³ d ⁻¹]
Rnp	net primary production rate [gC m ⁻³ d ⁻¹]
$Rrsp$	respiration rate [gC m ⁻³ d ⁻¹]

Remarks:

- ◇ The rates of the effects on the mass balances of dissolved oxygen, nutrients and detritus are simply derived from the above rates by multiplication with stoichiometric constants.
- ◇ The nutrient constraints are the minimal value of the quantities of available inorganic nutrients divided by the relevant algal stoichiometric constant. Only one nutrient at a time can be limiting to the growth of algae.
- ◇ Some algae species can satisfy a part of their nutrient demands by the consumption of organic detritus. Other algae species are capable of the fixation of dissolved elementary nitrogen. The effects of respectively mixotrophy and nitrogen fixation are included in the nutrient constraints, respectively by adding the nutrients available in detritus or in an indefinite stock of elementary nitrogen.
- ◇ The light limitation function can be based on daily average and depth average conditions. This function is associated with the critical ambient extinction coefficient which is species specific. The coefficient is derived from imposed tables that relate production efficiency to ambient light intensity (irradiation). Growth inhibition if the radiation is larger than the optimal radiation may be included in these tables. The tables are part of the BLOOM data base.
- ◇ The advantage of buoyancy of certain (blue green) algae species can be taken into account by means of a depth corrected light limitation function.
- ◇ Macro algae like *Ulva* attached to the sediment can be simulated as a phytoplankton species by means of non-transportability and a depth corrected light limitation function.
- ◇ Growth respiration is included in the potential production rate because of the biomass maximisation principle. Nutrients released as the consequence of respiration will quickly be taken up again in order to achieve maximal biomass production.
- ◇ Autolysis takes care that a certain fraction of the nutrients tied up in biomass is released as inorganic nutrients at the mortality of algae. The remaining fraction is added to various detritus pools. The fractionating is species specific.

- ◇ The excretion of organic matter (nutrients) by algae is ignored.
- ◇ BLOOM may also take into account sulphur from SO₄, in which case it turns over sulphur into POS1-2 at mortality. However, sulphur is not limiting phytoplankton growth.
- ◇ BLOOM may also be limited by carbon dioxide modelled as (TIC).

Phytoplankton: DYNAMO

The gross primary production for DYNAMO follows from:

$$R_{gp_i} = f_{nut_i} \times f_{lt_i} \times k_{gp_i} \times C_{alg_i}$$

with:

C_{alg}	algal biomass concentration [gC m ⁻³]
f_{lt}	light limitation factor [-]
f_{nut}	nutrient limitation factor according to Monod [-]
k_{gp}	potential gross primary production rate [d ⁻¹]
R_{gp}	gross primary production rate [gC m ⁻³ d ⁻¹]
i	index for species group (Diat or Green) [-]

The nutrient limitation factor for DYNAMO considers only the most limiting nutrient:

$$f_{nut_i} = \min \left(\frac{C_n}{K_{sn} + C_n}, \frac{C_{ph}}{K_{sph} + C_{ph}}, \frac{C_{si}}{K_{ssi} + C_{si}} \right)$$

with:

C_n	ammonium plus nitrate concentration [gN m ⁻³]
C_{ph}	phosphate concentration [gP m ⁻³]
C_{si}	dissolved inorganic silicate concentration [gSi m ⁻³]
K_{sn}	half saturation constant for nutrient nitrogen [gN m ⁻³]
K_{sph}	half saturation constant for phosphate [gP m ⁻³]
K_{ssi}	half saturation constant for silicate [gSi m ⁻³]

The light limitation function for DYNAMO is a combination of a day length factor and a radiation limiting factor that saturates for day length and light intensities larger than the optimal day length and light intensity:

$$f_{lt_i} = f(I_z, I_{o_i}, DL, DLo_i, \dots)$$

with:

DL	day length [d]
DLo	optimal day length [d]
f_{lt}	light limitation factor [-]
I_z	depth average light intensity in a water layer [W m ⁻²]
I_o	optimal light intensity [W m ⁻²]

The depth averaged light intensity is derived according to Lambert-Beer's Law for light attenuation:

$$I_z = I_{top} \times e^{(-ec \times z)}$$

with:

ec	extinction coefficient of visible light [m ⁻¹]
I_{top}	light intensity at the top of a water layer [W m ⁻²]

z water depth [m]

The extinction coefficient is the sum of contributions of the background (water plus not modelled substances), live algae biomass, particulate and dissolved detritus and inorganic suspended matter. These contributions follow from the multiplication of concentrations and specific extinction coefficients.

The rates of respiration and mortality in DYNAMO are described with:

$$Rrsp_i = krsp_i \times Calg_i + frsp_i \times Rgp_i$$

$$Rmrt_i = kmrt_i \times Calg_i$$

$$kmrt_i = f(Ccl, T)$$

with:

Ccl	chloride concentration [g m^{-3}]
$frsp$	fraction of gross production respired [-]
$kmrt$	total mortality process rate [d^{-1}]
$krsp$	maintenance respiration rate [d^{-1}]
$Rmrt$	total mortality rate [$\text{gC m}^{-3} \text{d}^{-1}$]
$Rrsp$	total respiration rate [$\text{gC m}^{-3} \text{d}^{-1}$]

Remarks:

- ◇ There is no growth inhibition if the radiation is larger than the optimal radiation.
- ◇ Autolysis takes care that a certain fraction of the nutrients tied up in biomass is released as inorganic nutrients at the mortality of algae. The remaining fraction is added to various detritus pools. The fractionating is species specific.
- ◇ The excretion of organic matter (nutrients) by algae is ignored.

6.9 Primary consumption

6.9.1 Concepts

One module (CONSBL) is available for the modelling of primary consumers such as zooplankton and zoobenthos. These primary consumers are also indicated as grazers. CONSBL is described with respect to organic carbon and nutrients incorporated in the organisms or affected by them. The nutrients concern nitrogen, phosphorus and silicon. The description of the consumer modules includes the uptake of phytoplankton biomass and detritus for food, the production, respiration and mortality of biomass, and the excretion of detritus and nutrients. The effects of consumers on dissolved oxygen by means of respiration are ignored.

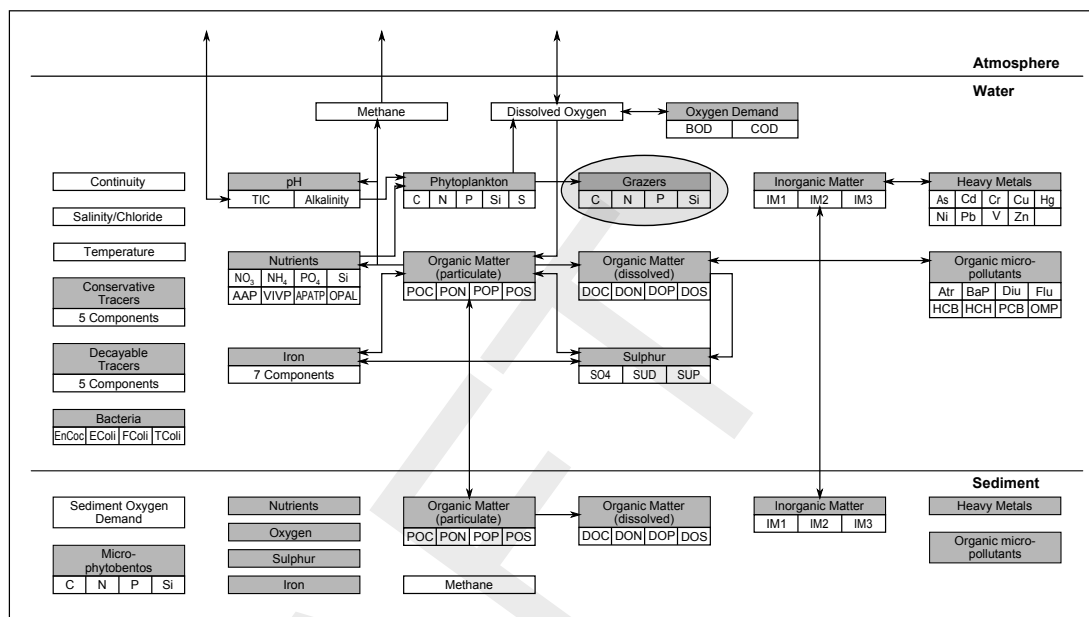


Figure 6.8: Overview of substances. Primary consumption

The modelling of all other processes to which the nutrients and detritus are subjected are described in [section 6.7](#) of this manual. [section 6.8](#) provides the description of the modelling of phytoplankton processes.

Pelagic and benthic grazing pressure can be imposed on the model as a forcing function with module CONSBL (WL | Delft Hydraulics, 1990). This module can be applied for up to five types of grazers, which may be species groups or individual species of zooplankton and zoobenthos. CONSBL requires that biomasses of grazers are imposed to the model as time-series. Imposed biomasses will be adjusted, if constraints for growth, mortality and available food are exceeded. Using the grazer biomass time-series as boundary conditions CONSBL generates the mass fluxes due to grazing with respect to algae biomass, detritus and nutrients in a consistent and mass conservative way.

The advantage of a forcing function over a dynamic grazing model is that the grazer biomass is controlled. Even state-of-the-art dynamic simulation of grazers is still subjected to problems concerning stability and limited accurateness. However, imposing forcing functions demands for reliable and rather frequently measured grazer biomass data.

6.9.2 Modelling framework

CONSBL imposes the grazing pressure of up to five species (groups) of zooplankton and zoobenthos. The names of the input parameters for biomass are:

Name of D-Water Quality substance	Description	Unit
Zooplank	Zooplankton	gC/m^3
Mussel	Mussels	gC/m^2
Grazer3	Optional user-defined 3rd grazer	gC/m^3 or gC/m^2

Name of D-Water Quality substance	Description	Unit
Grazer4	Optional user-defined 4th grazer	gC/m ³ or gC/m ²
Grazer5	Optional user-defined 5th grazer	gC/m ³ or gC/m ²

Although input parameter names of the first two groups refer to respectively zooplankton and mussels (zoobenthos), you still need to define the nature of each of the groups. The grazer biomass in CONSBL is subjected to growth or mortality, and to growth and maintenance respiration. The imposed biomass is corrected in order to obey constraints for growth, mortality and food availability. The grazer process rates are transformed into the rates of the consumption of detritus and algae, and the production of detritus and inorganic nutrients. According to the specification a fraction of the produced detritus is added to the sediment detritus pools, whereas the remainder is allocated to detritus in the water column.

The assumptions for forcing function CONSBL are:

- 1 Grazers in the water column and at the sediment have essentially the same behaviour in terms of food consumption, growth, respiration, mortality and detritus production. They are different in the sense that detritus produced is released into the water column and/or deposited at the sediment.
- 2 The existence of distinct physiological types within a grazer species can be ignored.
- 3 Grazers are not subjected to settling and resuspension.
- 4 Grazers consume algae species and detritus for food. Grazer species are different with respect to their preference for these food components.
- 5 Nutrient-carbon ratios in grazer species are constant and species specific, consequently nutrients are taken up by grazers in constant ratios. The same holds for the release of organic nutrients due to mortality.
- 6 Grazers produce detritus due to egestion of a part of the ingested food as fecal pellets, and due to mortality. The surplus is determined for every organic nutrient (C, N, P, Si) as the sum of poorly digestible food fractions and the excess nutrient intakes. The fractions are specific for both food components and grazer species. Most grazers do not use silicon at all.
- 7 Grazers produce inorganic nutrients due to respiration.
- 8 The change of grazer biomass during a time step can not be larger than constraints for maximal growth or maximal mortality, and for available food. Growth and mortality do not necessarily concur. The imposed grazer biomass is adjusted in accordance with these constraints.
- 9 Maximal growth is proportional to the biomass concentration and a maximal growth rate. Maximal mortality is proportional to the biomass concentration and a maximal mortality rate.
- 10 Respiration is the sum of growth respiration and maintenance respiration. Growth respiration is a species specific fraction of gross production. Maintenance respiration is proportional to the algal biomass and a respiration rate.
- 11 Grazer maximal growth, respiration and maximal mortality rates are functions of temperature with a species specific coefficients.
- 12 Actual growth is equal to the net increase of grazer biomass over a time step. Net food assimilation is equal to the net increase of grazer biomass plus respiration.
- 13 Actual mortality is equal to the net decrease of grazer biomass over a time step plus. Net detritus production is equal to mortality minus respiration.

- 14 Grazer consumption is proportional to the biomass concentration and a grazer consumption rate. This rate is either equal to the maximal uptake rate or to a filtration rate. Both are temperature dependent and grazer species specific. The rate applied depends on the exceedence of a critical food concentration, which is the concentration for which the rates are equal. The filtration rate is formulated according to Monod kinetics.
- 15 The autolysis of grazer biomass at mortality can be ignored.

6.9.3 Process equations

Grazing: CONSBL

The form of the formulations of forcing function module CONSBL deviates strongly from the form in dynamic producer and consumer modules because the grazer biomass is imposed instead of predicted. The consumption rates for algae and detritus are deduced from the change of grazer biomasses over a time step. However, this change must be consistent with maximal growth or maximal mortality, and with the available food. Consequently, the imposed biomass is adjusted when one of these constraints is not met. The growth, mortality and food constraints are respectively:

$$Cgrc_i = \begin{cases} Cgr1_i \times (1 + kgr_i \times \Delta t) & \text{if } Cgr2_i \geq Cgr1_i \\ Cgr1_i \times (1 - kmrt_i \times \Delta t) & \text{if } Cgr2_i < Cgr1_i \end{cases}$$

with:

$Cgr1_i$	grazer biomass concentration at t_1 [gC m ⁻³]
$Cgrc_i$	grazer biomass concentration constraint at t_2 [gC m ⁻³]
kgr	maximal growth rate [d ⁻¹]
$kmrt$	maximal natural mortality rate [d ⁻¹]
Δt	time step [d]
i	index for grazer species group 1–5 [-]
k	index for nutrients, 1 = carbon, 2 = nitrogen, 3 = phosphorus, 4 = silicon [-]

The available food is equal to the sum of component concentrations multiplied with preference parameters that can be considered weight factors:

$$Cfd_i = fdpr_i \times Cdet_1 + \sum_{j=1}^m (fapr_i \times Calg_j)$$

with:

$Calg_j$	biomass concentration of algae species group j [gC m ⁻³]
Cfd_i	food concentration available to grazer species group i [gC m ⁻³]
$Cdet_i$	detritus organic carbon concentration [gC m ⁻³]
$fdpr_i$	preference of a grazer species group i for detritus [-]
$fapr_{i,j}$	preference of a grazer species group i for algae species group j [-]
m	number of algae groups [-]
j	index for algae species groups [-]

The consumption rates for detritus and algae biomass of a grazer group are:

$$\begin{aligned} Rdcns1_{k,i} &= fdpr_i \times kcns_i \times Cdet_k \\ Racns_{k,i,j} &= fapr_{i,j} \times kcns_i \times anut_{k,j} \times Calg_j \end{aligned}$$

with:

$anut_{k,j}$	stoichiometric const. of nutrient k over organic carbon in algae j [gC/N/P/Si gC ⁻¹]
--------------	--

$Cdet_k$	detritus concentration for nutrient k [gC/N/P/Si m ⁻³]
$fdpr_i$	preference of a grazer species group i for detritus [-]
$fapri,j$	preference of a grazer species group i for algae species group j [-]
$kcns_i$	consumption process rate of grazer group i [d ⁻¹]
$Racns_{k,i,j}$	cons. rate of grazer group i for nutrient k in algae j [gC/N/P/Si m ⁻³ d ⁻¹]
$Rdcns1_{k,i}$	gross cons. rate of grazer group i for nutrient k in detritus [gC/N/P/Si m ⁻³ d ⁻¹]

The consumption process rate is equal to either the maximal uptake rate or a filtration rate depending on whether the available concentration of food is larger or smaller than a certain critical amount. This amount is the biomass concentration for which the filtration rate and the maximal uptake rate are equal.

Consumed food is either assimilated as grazer biomass, respired or egested as detritus (faecal pellets). Depending on the nature of the grazer group a part of the egested detritus is deposited at the sediment and is therefore added to the sediment detritus pool. The total rates of food assimilation, net detritus consumption and sediment detritus production caused by grazing are as follows:

$$\begin{aligned}
 Ras_{k,i} &= (1 - fdet_i) \times Rdcns_{k,i} + \sum_{j=1}^m ((1 - falg_{i,j}) \times Racns_{k,i,j}) \\
 Rdcns2_{k,i} &= (1 - fdet_i) \times Rdcns1_{k,i} + \sum_{j=1}^m ((1 - falg_{i,j} \times (1 - fsed_i)) \times Racns_{k,i,j}) \\
 Rsdpr_{k,i} &= fdet_i \times fsed_i \times Rdcns1_{k,i} + \sum_{j=1}^m (falg_{i,j} \times fsed_i \times Racns_{k,i,j})
 \end{aligned}$$

with:

$falg_{i,j}$	egested fraction of algae j consumed by grazer i , =1-yield [-]
$fdet_i$	egested fraction of detritus consumed by grazer i , =1-yield [-]
$fsed_i$	fraction of detritus egested by grazer i added to the sediment detritus pool [-]
$Ras_{k,i}$	total food assimilation rate for nutrient k for grazer group i [gC/N/P/Si m ⁻³ d ⁻¹]
$Rdcns2_{k,i}$	net cons. rate of grazer group i for nutrient k in detritus [gC/N/P/Si m ⁻³ d ⁻¹]
$Rsdpr_{k,i}$	total nutrient k in detr. prod. at the sediment for all grazers [gC/N/P/Si m ⁻³ d ⁻¹]

The rates are corrected for nutrient limitation, respiration and the change of grazer biomass resulting from the food constraint. The nutrient limitation leads to a decrease of $Rdcns$ and an increase of $Rsdpr$ for those nutrients in the food that are available in excess as calculated on the basis of grazer biomass stoichiometry. Respiration causes a decrease of both rates and the release of equivalent amounts of inorganic nutrients. The growth and maintenance respiration rates are described with:

$$Rrsp1_{k,i} = bnut_{k,i} \times frsp1_i \times Ras_{1,i}$$

$$Rrsp2_{k,i} = bnut_{k,i} \times krsp2_i \times Cgr1_i$$

with:

$bnut_{k,i}$	stoichiometric const. of nutrient k over organic carbon in grazer i [gC/N/P/Si gC ⁻¹]
$frsp1_i$	growth respiration fraction [-]
$krsp2_i$	maintenance respiration rate [d ⁻¹]
$Rrsp1_{k,i}$	growth respiration rate for nutrient k and grazer i [gC/N/P/Si m ⁻³ d ⁻¹]
$Rrsp2_{k,i}$	maintenance respiration rate for nutrient k and grazer i [gC/N/P/Si m ⁻³ d ⁻¹]

Finally, in case of mortality the grazer biomass decrease over a time step is allocated to the detritus production rates.

6.10 Heavy metals and organic micro-pollutants

6.10.1 Concepts

Two types of micropollutants can be modelled with D-Water Quality: heavy metals and organic micro-pollutants. These types of pollutants show conformities but also many basic differences with respect to properties and processes. Both conformities and major differences have been taken into account in D-Water Quality.

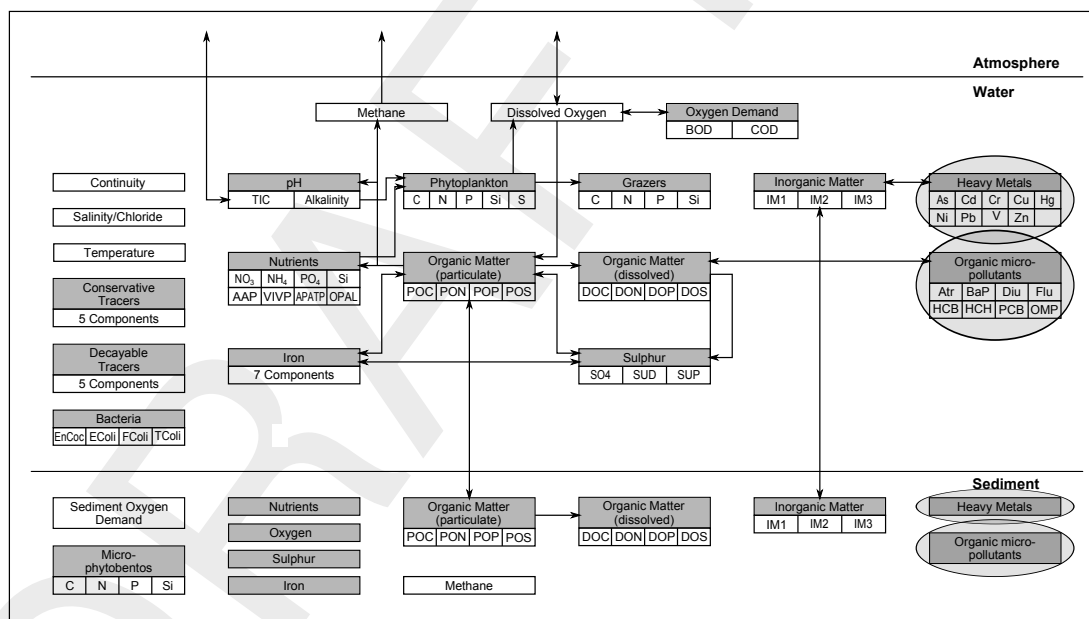


Figure 6.9: Overview of substances. Heavy metals and organic micro-pollutants

Because the fate of most micropollutants is largely determined by the adsorption to particulate matter, suspended inorganic and organic matter (including phytoplankton) has to be included in the model in most cases. It may be necessary to include dissolved organic matter as well.

In D-Water Quality the two options available for sediment-water interaction and return fluxes, the layered sediment approach and the S1-S2 approach, are also applicable for the modelling of micropollutants.

6.10.2 Modelling framework

Heavy metals

The heavy metals that can be modelled are divided among three subgroups:

Name of D-Water Quality substance	Description	Unit
<i>Group 1: sulphide-forming heavy metals</i>		
Cd	Cadmium	g/m ³

Name of Water substance	D-Quality	Description	Unit
Cu		Copper	g/m ³
Pb		Lead	g/m ³
Hg		Mercury	g/m ³
Ni		Nickel	g/m ³
Zn		Zinc	g/m ³
<i>Group 2: hydroxide-forming heavy metals</i>			
Cr		Chromium	g/m ³
<i>Group 3: heavy metals occurring as anions</i>			
As		Arsenic	g/m ³
Va		Vanadium	g/m ³

Strictly speaking, vanadium and arsenic do not belong to the group of heavy metals. Group 1 encompasses the heavy metals that tend to form poorly soluble sulphides at chemically reducing conditions. Chromium and arsenic do not form sulphide precipitates under normal conditions in sediments. However, chromium and vanadium may form (hydr)oxides. Arsenic and vanadium are present as anions, whereas the other metals form free or complexed cations in the solution. Referring to their ionic state, some of the metals can possess more than one valency. Although dependent on the chemical conditions to some extent, one valency is usually dominant over the other valencies at prevailing natural conditions. The differences between the groups of metals have important consequences for the partitioning of the metals among several dissolved and particulate phases.

Metals are conservative substances. The fate of heavy metals in a water system is determined primarily by partitioning to water and particulate matter (including phytoplankton), and by transport. The partitioning divides the total amount of a pollutant into a 'dissolved' fraction and several 'adsorbed' fractions. Adsorbed fractions of a metal are influenced by all the processes that affect particulate matter, such as settling, resuspension, burial and digging.

Partitioning of metals is described in general by:

- 1 sorption to particulates;
- 2 precipitation in minerals; and
- 3 complexation in solution.

Complexation with inorganic and organic ligands can be considered implicitly in partitioning by using reprofuctions for the partitioning coefficient. Sorption can be modelled as an equilibrium process (equilibrium partitioning) or as the resultant of slow adsorption and desorption reactions (kinetic formulations). In the latter case, partitioning is assumed to proceed at a finite rate proportional to the difference between the actual state and the equilibrium state. D-Water Quality uses one state variable (substance name) for equilibrium sorption, which represents the total metal concentration. Alternatively, D-Water Quality uses two state variables (substance names with name additions -Dis and -Par) for slow sorption, one for the dissolved metal concentration and one for the particulate metal concentration.

To describe the fate of certain heavy metals in reducing environments, such as sediment layers, the formation of metal sulphides or (hydr)oxides can be modelled. The soluble metal concentration is determined on the basis of the relevant solubility product. The excess metal is stored in a precipitated metal fraction.

Notice that sorption and precipitation affect the dissolved metal concentration in different ways. Both the adsorbed and dissolved fractions increase at increasing total concentration, as long as no solubility product is exceeded. The dissolved concentration is bounded by precipitation at the level at which a solubility product is exceeded.

Mercury is modelled like cadmium. Organic forms (methylated species) are ignored, which can be justified from the quantitative point of view. The methylated forms of lead and arsenic have not been taken into consideration for similar reasons.

Metals such as silver, cobalt, antimony, selenium and molybdenum have not been mentioned, but can be modelled approximately as one of the other metals.

Assumptions for heavy metals:

- 1 Heavy metals can adsorb to particulate inorganic matter (up to three fractions), to dead particulate and dissolved organic matter (up to five fractions), and to phytoplankton (sum of various algae species).
- 2 The adsorption to particulate matter and dissolved organic matter is described by means of equilibrium or kinetic partitioning, on the basis of partitioning coefficients. For each particulate phase, a different partition coefficient is defined. A total of 5 partition coefficients must be provided if all particulate fractions are present in the model (K_{pim1-3} , K_{ppoc} and K_{palg} respectively). In case DOC is modelled as well, an additional coefficient is needed.
- 3 The partition coefficient is in fact a function of the macrochemical composition of the water (pH and various ions) and the macrochemical composition of the inorganic matter (binding capacity). These dependencies can be taken into account in the reprofuction for the partitioning coefficient.
- 4 Complexation of metals in solution can be considered implicitly in so-called repro-functions for the partition coefficient. Complexation is also considered implicitly in precipitation equilibria. Relevant ligands are hydroxyl, bicarbonate, chloride and sulphides.
- 5 All metal is assumed to be available for partitioning.
- 6 The precipitation of metal sulphides is described as equilibrium process, on the basis of a solubility product. Precipitation depends on the presence of dissolved oxygen, which has to be imposed as forcing function, or has to be simulated. The pH and the total dissolved sulphide concentration have to be provided as well. It is assumed that sulphide is always present in abundance, so that all particulate metal is in the metal sulphides.
- 7 The precipitation of metal (hydr)oxides is described as equilibrium process, on the basis of a solubility product. The pH has to be provided. First the metal is divided among dissolved and adsorbed species in agreement with the solubility product. Next the remaining metal is stored in (hydr)oxides.
- 8 The partitioning processes are different for the sulphide forming metals in reducing and oxidising environments.
- 9 Arsenic and vanadium are not subjected to precipitation. Adsorption in the reducing environment is described in the same way as in the oxidising environment.
- 10 Some metals, mercury in particular, are subject to methylation by microbes. Organic mercury species are important from a bioaccumulation point of view, but little important in terms of chemical speciation (WL, 1991). Quantification of the processes concerned is still difficult, so formulations for these processes have not been implemented.
- 11 Volatization is ignored for all heavy metals, even for mercury, because it is negligible.

Organic micro-pollutants

Principally, all organic micro-pollutants can be modelled with substance OMP, a number of substances have been defined in D-Water Quality allowing for joint simulation.

Name of D-Water Quality substance	Description	Unit
OMP	(general) Organic Micro-Pollutant	g/m ³
HCH	Hexachlorohexane (γ -HCH or lindane)	g/m ³
HCB	Hexachlorobenzene	g/m ³
153	PCB-153	g/m ³
BaP	Benzo-a-pyrene	g/m ³
Flu	Fluoranthene	g/m ³
Diu	Diuron	g/m ³
Mef	Mevinfos	g/m ³
Atr	Atrazine	g/m ³

The short term fate of organic micropollutants in a water system is determined primarily by partitioning to water and particulate and dissolved organic matter (including phytoplankton), and by transport. Refer to the heavy metals for more details regarding transport and adsorption, which can be described according to equilibrium partitioning or slow kinetics.

Organic micropollutants are also influenced by additional processes such as volatilisation and degradation. Various (bio)chemical degradation processes can be distinguished, but present D-Water Quality only considers overall degradation. The rates of these processes are concentration and temperature dependent.

The presence of a micropollutant in a water system is described by the total concentration (sum of dissolved and particulate concentrations), the total particulate concentration and the total dissolved concentration for each water and sediment compartment. The particulate and dissolved concentrations are derived from the total concentration and the respective fractions. The latter are calculated from partitioning formulations.

Assumptions for organic micropollutants:

- 1 Organic substances adsorb to particulate and dissolved detrital organic matter (up to five fractions), to phytoplankton biomass (sum of the biomass of various algae species).
- 2 The adsorption to particulate matter is described by means of equilibrium or kinetic partitioning, on the basis of a partitioning coefficient (K_{ppoc} and K_{palg} respectively). Adsorption to dissolved organic matter (DOC) is described indirectly, by means of the partitioning coefficient for particulate organic carbon (K_{ppoc}) and an efficiency factor (X_{doc}).
- 3 The partition coefficient is in fact a function of the pH when ionic substances are concerned. This dependency has been neglected in the model.
- 4 All organic micropollutant is available for partitioning.
- 5 Transport of organic micropollutants across the water-atmosphere interface (e.g. volatilisation) is based on the double film theory. Equilibrium is assumed between the concentrations of the micropollutant in the gas film and the liquid film according to Henry's Law. Only the free dissolved micropollutant is available for volatilisation.

- 6 Three types of degradation processes can be distinguished: photolysis, hydrolysis and biodegradation. For all processes the degradation rate is proportional to the micropollutant concentration, and a function of temperature. The photolysis rate is also dependent on solar radiation. The hydrolysis rate is dependent on the pH. The biodegradation constants are dependent on the presence of oxidising or reducing conditions, e.g. the presence of dissolved oxygen. The formulations for the individual degradation processes have not (yet) been made operational in standard D-Water Quality.
- 7 The various processes for decomposition of organic micropollutants are integrated in one overall degradation process. First order temperature dependent kinetics have been used to formulate this process. Different degradation rate constants can be provided to water and sediment compartments.
- 8 By means of an option parameter the various dissolved fractions or the total concentration can be subjected to degradation.

General assumptions:

- 1 For the S1-S2 approach of the sediment-water interaction the substances of the heavy metals and the organic micro-pollutants in the water column settle in the same substances in the sediment, but S1 or S2 are added in the names of the substances in the sediment.
- 2 The rates of settling, resuspension, burial and digging of micropollutants are proportional to the rates for particulate inorganic matter (sediment).

6.10.3 Process equations

The mass balance equations read:

(for water)

$$\frac{\Delta Ct}{\Delta t} = \text{loads} + \text{transport} + \text{resuspension} - \text{settling} - \text{losses}$$

(for sediment)

$$\begin{aligned} \frac{\Delta Ct}{\Delta t} = & +\text{settling} - \text{resuspension} + \text{digging} - \text{burial} \pm \text{bioturbation} \\ & \pm \text{dispersion(bioirrigation)} \pm \text{seepage} - \text{losses} \end{aligned}$$

with:

Ct	total concentration of a micropollutant [g m^{-3}]
t	time [day]

The term '*transport*', representing advection and dispersion, is always present when two or more water compartments are considered. When a micropollutant partitions among particulate and dissolved phases, this term affects all phases equally. It is obvious that all other specifically particle related transport processes disappear from the equation for non-adsorbing (i.e. dissolved phase) micropollutants.

Whereas D-Water Quality simulates total concentration (mass in fact) in compartments, the particulate and dissolved fractions are needed for this purpose. The rates of transport processes that affect only the particulate or only the dissolved parts of a micropollutant are corrected with these fractions. They are also used to produce output on the magnitude of the particulate and dissolved concentrations.

The fractions are calculated with the following typical equations:

$$Ct = (fim + fpoc + fdoc + falg + fd) \times Ct$$

$$fd = \frac{\phi}{\phi + Kpim \times Cim + Kppoc \times (Cpoc + Xdoc \times Cdoc) + Kpalg \times Calg}$$

$$fim = (1 - fd) \times \frac{Kpim \times Cim}{Kpim \times Cim + Kppoc \times (Cpoc + Xdoc \times Cdoc) + Kpalg \times Calg}$$

$$fpoc = (1 - fd) \times \frac{Kppoc \times Cpoc}{Kpim \times Cim + Kppoc \times (Cpoc + Xdoc \times Cdoc) + Kpalg \times Calg}$$

$$fdoc = (1 - fd) \times \frac{Xdoc \times Kppoc \times Cpoc}{Kpim \times Cim + Kppoc \times (Cpoc + Xdoc \times Cdoc) + Kpalg \times Calg}$$

$$falg = (1 - fd - fim - fpoc - fdoc)$$

with:

$Calg/im/poc$	concentration of algae biomass [gC m ⁻³] inorganic matter, [gDW m ⁻³]
Ct	dead particulate organic matter [gC m ⁻³]
$falg/im/poc/doc$	fraction of a micropollutant adsorbed to algae biomass, inorganic matter, detrital particulate organic matter, dissolved organic matter [-]
fd	dissolved fraction of a micropollutant [-]
$Kpalg/im/poc$	partition coefficient for algae [m ³ gC ⁻¹] inorganic matter [m ³ gDW ⁻¹]
$Xdoc$	detrital particulate organic matter [m ³ gC ⁻¹]
ϕ	efficiency (attenuation) factor for partition coefficient for dissolved organic matter [-]
ϕ	porosity [m ³ water m ⁻³]

The partitioning coefficient is generally defined as follows:

$$Kp = \frac{Cp'}{Cd'} = \frac{\phi \times Cp}{Cs \times Cd} \times 10^6$$

with:

Kp	equilibrium partition coefficient [mg.kg ⁻¹ DW/mg l ⁻¹ water]
Cd'	dissolved concentration of a micropollutant [mg l ⁻¹ water]
Cp'	particulate concentration of a micropollutant [mg.kg ⁻¹ DW] or [mg kg ⁻¹ C]
Cd	dissolved concentration of a micropollutant [mg m ⁻³]
Cp	particulate concentration of a micropollutant [mg m ⁻³]
Cs	concentration of particulate matter [gDW m ⁻³] or [gC m ⁻³]

Differences in the equations for the various types of micropollutants arise in relation to specific affinities to either inorganic matter and/or organic matter and in relation to speciation in solution.

Partitioning can be simulated according to the above equilibrium approach (option 1) or according to slow sorption kinetics (option 2). Option 1 generates a sorption flux as the difference between the end concentration of the previous time step and the equilibrium concentration of the actual time step, divided by the time step Δt . For option 2 the sorption flux follows from:

$$Rsorp = ksorp \times (Cpe - Cp)$$

with:

C_p	actual particulate concentration of a micropollutant [mg m^{-3}]
C_{pe}	equilibrium particulate concentration of a micropollutant [mg m^{-3}]
k_{sorp}	first order kinetic constant for adsorption and desorption [d^{-1}]
R_{sorp}	rate of adsorption or desorption [$\text{mg m}^{-3} \text{d}^{-1}$]

The equilibrium concentration of the adsorbed micropollutant can be calculated from the above fractions and the total concentration. Option 2 can be linked up with option 1 by solving the equation as an exponential equation for time step Δt , and by feeding the resulting concentration into the concentration difference of option 1 instead of the equilibrium concentration.

The mass balance equations are basically similar for all micropollutants except for the loss processes. Below the differences are illuminated for each group of micropollutants.

Heavy metals

In principal the speciation in solution can be taken into account in adsorption using so-called repro-functions for the partition coefficients. The repro-functions demand for information on the cation exchange capacity (CEC) of the inorganic matter, the pH and the concentrations of various ligands.

The adsorption of arsenic is treated a little differently from that of other metals. Arsenic, present as AsO_4^{3-} , adsorbs specifically to organic matter and to oxidised iron in inorganic matter. Consequently, the latter sorption component disappears under reducing conditions. This could be taken into account in the model by formulating the partition coefficient as a function of the reactive, oxidized iron content in the inorganic matter. This content would have to be imposed as forcing function for all water and sediment components. Providing $\%Fe = 0.0$ to a sediment compartment would lead to $K_{pim} = 0.0$ for that compartment. However, this option has not yet been included in standard D-Water Quality.

In order to take precipitation into account partitioning is modified. In case of metal sulphides precipitation can only occur when dissolved oxygen is not present. So D-Water Quality checks the dissolved oxygen concentration for each compartment, which requires that dissolved oxygen be imposed, for instance as a forcing function. The algorithm for precipitation is basically as follows. First the total dissolved metal concentration is calculated from a constant solubility product and the stability constants of various metal complexes. A solubility product is the product of the free metal ion concentration and the concentration(s) of the relevant anion(s). A stability constant provides the ratio between the free metal ion concentration multiplied with the concentration of a ligand, and the concentration of a metal complex. The pH and the total dissolved sulphide concentration are inputs for the calculations (forcing functions). The metal not dissolved is entirely allocated to the sulphide.

For metal hydroxides the metal is adsorbs proportional to the equilibrium dissolved concentration, whereas the remaining part is stored in the precipitated fraction.

Organic micro-pollutants

The adsorption of organic micropollutants is described the same equations as for heavy metals. However, organic micropollutants only adsorb to organic matter, including dissolved organic matter. The fraction adsorbed to dissolved organic matter (DOC) is calculated with the partition coefficient for particulate detrital organic matter (POC) multiplied with efficiency (attenuation) factor $X_{doc} (\leq 1)$.

Loss processes for organic micropollutants are volatilization, biodegradation, photolysis and hydrolysis. The three degradation processes have been lumped into one overall degradation process in standard D-Water Quality. Basically all these processes have been formulated according to first order kinetics. However, some of the kinetic constants are pseudo first order constants, since they are in fact functions of other state variables, imposed on the model as forcing functions.

Volatilization is formulated according to the double film theory. The volatilisation rate is equal to:

$$R_{vol} = -\frac{F_{vol}}{H} = -\frac{k_{vol} \times Cd}{H}$$

with:

Cd	dissolved concentration of a micropollutant [mg m^{-3} water]
F_{vol}	volatilisation mass flux [$\text{mg m}^{-2} \text{d}^{-1}$]
H	water depth or thickness of the upper water layer [m]
k_{vol}	overall transfer coefficient for volatilization [m d^{-1}]
R_{vol}	volatilisation rate [$\text{mg m}^{-3} \text{d}^{-1}$]

This equation is only valid when the atmospheric concentration is negligibly small, which it always is the case. The overall transfer coefficient is composed of contributions of the transfer coefficients of the liquid layer and gas layer bordering the water atmosphere interface. It is also a function of Henry's constant, defined as the ratio of the atmospheric concentration and the dissolved concentration in equilibrium. The partial transfer coefficients are calculated from the wind speed and various properties of water and air. Both Henry's constant and the transfer coefficient are functions of the temperature.

All other loss processes are basically described with:

$$R = -k \times Ct$$

with:

Ct	total concentration of a micropollutant [mg m^{-3}]
k	(pseudo) first order kinetic constant for overall degradation [d^{-1}]
R	rate of overall degradation [$\text{mg m}^{-3} \text{d}^{-1}$]

Overall degradation can be dominated by one the possible degradation processes: biodegradation, photolysis, oxidation, hydrolysis, etc. It can be shown that the degradation kinetics reduce to the above first-order kinetics assuming that various process parameters are more or less constant.

6.11 Sediment modelling

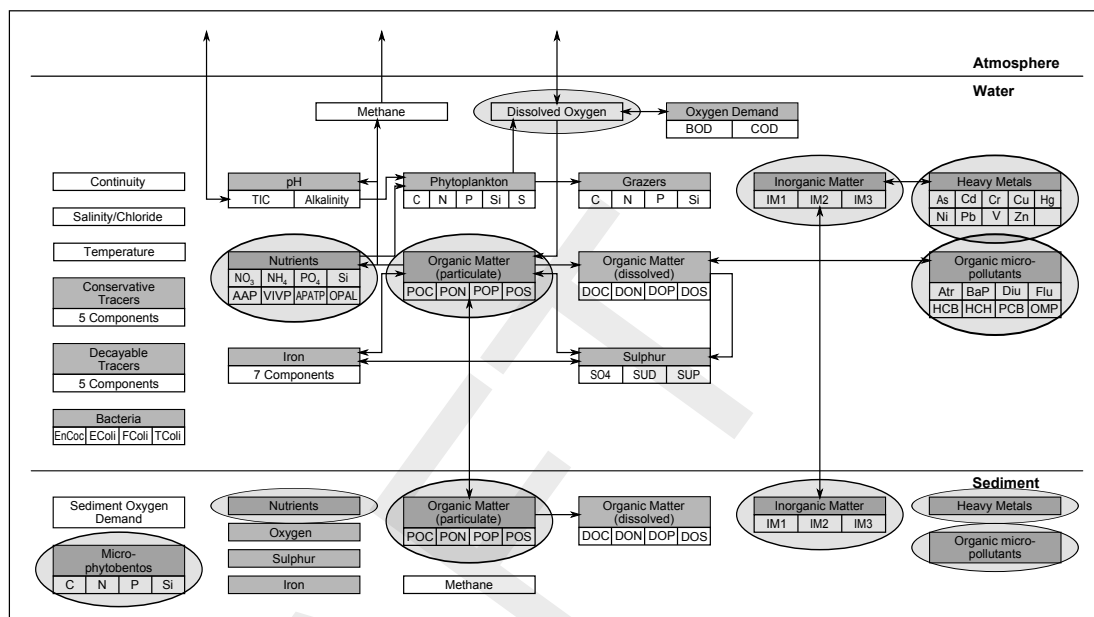


Figure 6.10: Overview of substances. Substances that are considered in the S1-S2 approach for sediment are encircled.

6.11.1 Concepts

The sediment is an important part of a water system. Not only is it a living environment for a whole range of specialised organisms, it can be either a sink for or a source of particulate and dissolved matter. The exchange of particulate and dissolved matter between the water column and the sediment can be of great importance for the water quality in the water column. Sediment-water interaction is usually included in water quality models, although often in simplified ways. In case of advanced water and sediment quality modelling sediment detailed simulation of the composition and diagenesis of the sediment may be included.

The principles of exchange of particulate matter between the water column and the sediment (i.e. settling-sedimentation and resuspension-erosion) are described in [section 6.6](#). This section focuses on sediment diagenesis and the exchange of dissolved substances between the water column and the sediment.

Physical aspects

Physically the sediment is characterised by the particulate fraction: grain size distribution, sediment strength and porosity. The porosity of freshly settled material can be very high (> 0.9), especially when the material consists of organic matter and clay particles ($< 63\mu\text{m}$). As more material settles on top, the pore water is gradually squeezed out by the building overlying pressure and the porosity decreases. Compacted sediment has a typical porosity of about 0.4.

(Bio)chemical aspects

The major driving force for (bio)chemical processes in the sediment is the mineralization of organic matter. Organic matter can be produced within the sediment through primary or secondary production or settled from the water column. The organic matter is worked into the sediment by bioturbation and burial. Various electron-acceptors are consumed for the oxidation of organic matter. Oxygen, nitrate, sulphate, manganese oxides (Mn(IV)), iron oxyhydroxides (Fe(III)), sulphate and carbon dioxide are subsequently consumed by bacteria as electron-acceptors. The final step when the other electron-acceptors are no longer available involves fermentation followed by the production of methane from carbon monoxide and hydrogen. This process is called methanogenesis. The reduced substances that arise from metal reduction, sulphate reduction and methanogenesis are oxidized with oxygen when diffusing upward to the aerobic top layer. The oxidation and reduction processes result in steep concentration gradients and chemically distinctive layers in the sediment, each layer having its dominant electron-acceptor. The aerobic top layer is usually less than a few millimeters thick. When going deeper in the sediment the aerobic top layer is successively followed by a denitrifying layer, an iron and sulphate reducing layer and a methanogenic layer. The redox potential decreases strongly from the sediment-water interface deeper into the sediment. In a model in view of modelling the composition of large inhomogeneous compartments processes overlap in the vertical direction. The nutrients nitrogen, phosphorus and silicon interact in different ways to the chemical conditions. The processes affecting the nutrients include nitrification, denitrification, adsorption, precipitation and dissolution, see [Table 6.11](#) for an overview. The stratified development of the composition of the sediment driven by the decomposition of organic matter is indicated as sediment diagenesis. Diagenesis results in the exchange of dissolved nutrients, electron-acceptors and reduced substances between sediment and overlying water. The exchange is established by dispersion (bio-irrigation, flow induced turbulence, diffusion) and often also by advection (seepage). The flux of oxygen from the water column into the sediment is called the sediment oxygen demand. The nutrient fluxes from the sediment into the overlying water are indicated as the nutrient return fluxes.

Whereas the adsorption of ammonium is weak and not sensitive for the redox potential this is totally different for the adsorption of phosphate. Iron oxyhydroxides are the most important adsorbent for phosphate in the sediment, and usually a large portion of total phosphorus is adsorbed. The iron oxyhydroxides are reduced in the reducing sediment layer implying that they can no longer adsorb phosphate. The adsorbed phosphate is released and a larger return flux may occur when the oxic top layer becomes thinner. When the top sediment layer becomes entirely reducing due to the mineralization of accumulated organic matter and inadequate transport of oxygen to the sediment, for instance in stratified water, the adsorption capacity of the sediment collapses and the return flux may increase very strongly. This has a large impact on water quality if phytoplankton is phosphorus limited.

Table 6.11: Major processes for ammonium, nitrate, phosphate and silica as occurring in sediment layers

Substances	Processes	Layers
Ammonium	<ul style="list-style-type: none"> ◇ mineralization of organic matter ◇ nitrification ◇ sorption 	<ul style="list-style-type: none"> ⇒ all layers ⇒ aerobic top layer ⇒ all layers

Process	Substances	Comments
Nitrate	<ul style="list-style-type: none"> ◇ nitrification ◇ denitrification 	<ul style="list-style-type: none"> ⇒ aerobic top layer ⇒ denitrifying layer
Phosphate	<ul style="list-style-type: none"> ◇ mineralization of organic matter ◇ sorption ◇ dissolution/precipitation of apatite P ◇ precipitation of vivianite P ◇ dissolution of vivianite P 	<ul style="list-style-type: none"> ⇒ all layers ⇒ strong in oxidizing layer ⇒ all layers ⇒ strong in reducing layers ⇒ aerobic top layer
Silica	<ul style="list-style-type: none"> ◇ dissolution opal 	<ul style="list-style-type: none"> ⇒ all layers

Biological aspects

Benthic organisms such as zoobenthos, microphytobenthos and rooted macrophytes may live at or in the sediment bed. Therefore, these organisms are very much dependent on the physical and chemical properties of sediments. However, the presence and activity of benthic organisms can also influence the physical and chemical properties and processes that take place within the sediment.

Benthic organisms can change the sediment stability and thus have effect on erosion/deposition processes by their potential effect on both the bed shear stress and the shear strength of the sediment. The bed shear stress is a combined effect of hydrodynamic conditions near the sediment and the bottom roughness. Higher plants such as seagrass decrease the current velocities thereby reducing the local erosion. Other organisms increase the bottom roughness by creating elevations and depressions at the sediment surface. This greater bottom roughness will increase the shear stress and thus has a negative effect on bottom stability. The shear strength of the sediment bed is increased by the excretion of polymeric substances by organisms such as epipellic diatoms, sticking the sediment particles together. The increased shear strength will stabilise the sediment. Organisms such as *Corrophium volutator* which graze on diatoms reduce the effect on sediment stability.

The chemical composition of and processes in the sediment are influenced even more by benthic organisms. This is the result of their metabolic processes (primary production, primary consumption and respiration) and their behaviour (sediment capturing, sediment reworking, tube building, etc.). Suspension feeders remove particles from the overlying water and deposit them on to the sediment. Deposit feeders ingest organic matter and sediment and return it to a different location in the sediment. This mixing of sediment by the activity of macrofauna is termed bioturbation. Zoobenthos transport water and solutes due to motion or ingestion, which is indicated with bio-irrigation. For instance, tube dwellers pump oxygenated water through their tubes into the anaerobic sediment. This creates a thin layer of oxidizing sediment around the tubes. Macrophytes leak oxygen from their roots in the reducing layers. The transport of substances by organisms may strongly affect chemical processes, composition and stratification in the sediment.

6.11.2 Modelling framework

D-Water Quality has two alternatives to simulate the sediment-water exchange of dissolved substances:

- 1 The S1-S2 approach
- 2 The layered sediment approach

The S1-S2 approach concerns the simplified sediment approach in D-Water Quality, which involves the simulation of so-called *inactive substances*. Inactive substances are only subjected to conversion processes and not to mass transport. Only particulate substances can be inactive in the S1/S2 option in D-Water Quality:

Name of D-Water Quality substance	Description	Unit
DetCS1/S2	Fast decomposing detrital carbon in layers S1 and S2	gC
DetNS1/S2	Fast decomposing detrital nitrogen in layers S1 and S2	gN
DetPS1/S2	Fast decomposing detrital phosphorus in layers S1 and S2	gP
DetSiS1/S2	Fast dissolving opal silicon in layers S1 and S2	gSi
OOCs1/S2	Slow decomposing detrital carbon in layers S1 and S2	gC
OONS1/S2	Slow decomposing detrital nitrogen in layers S1 and S2	gN
OOPS1/S2	Slow decomposing detrital phosphorus in layers S1 and S2	gP
OOSiS1/S2	Fast dissolving opal silicon in layers S1 and S2	gSi
AAPS1/S2	Adsorbed ortho-phosphate in layers S1 and S2	gP
DiatS1/S2	Diatoms in layers S1 and S2	gC
IM1S1/S2	Inorganic matter fraction 1 in layers S1 and S2	g
IM2S1/S2	Inorganic matter fraction 2 in layers S1 and S2	g
IM3S1/S2	Inorganic matter fraction 3 in layers S1 and S2	g
HMS1/S2	Heavy metal in layers S1 and S2 (cadmium, copper, lead, mercury, nickel, tin, zinc, chromium, arsenic and vanadium)	g
OMPS1/S2	Organic micro-pollutant in layers S1 and S2 (OMP, hexachlorohexane, hexachlorobenzene, PCB-153, Benzo-a-pyrene, Fluoranthene, Diuron, Atrazine and Mevinfos)	g

Given the generic process formulations, the substances and processes for the layered sediment option are exactly the same as the substances and the processes for the water column. Chemical conditions in the sediment such as the concentration of dissolved oxygen determine how processes turn out in the sediment. See Chapter 6 for substances, processes and the dependency on chemical conditions.

6.11.3 Process equations

In this section we deal with the process formulations for the S1-S2 option, and with mass transport in the sediment for the layered sediment approach. The generic formulations for all other processes in the layered sediment approach are discussed in [chapter 6](#). These formulations may turn out differently in the sediment depending on local chemical conditions, the dissolved oxygen concentration in particular. For the processes and formulations for organic matter, nutrients and electron-acceptors see [section 6.7](#). For phytoplankton see [section 6.8](#). For primary consumers (grazers) see [section 6.9](#). For heavy metals and organic micro-pollutants see [section 6.10](#). For the inorganic matter fractions see [section 6.6](#). The settling and resuspension of substances and how substances in the water column are allocated to substances in the sediment and vice versa for the S1-S2 option is also explained in these sections. Settled phytoplankton biomass dies in the sediment, instantly in the case of the S1-S2 approach, gradually in the layered sediment approach. Resuspended microphytobenthos biomass is turned over to the detritus pools in the water column instantly in the case of the S1-S2 approach.

The mass balance for all substances in the sediment according to the S1-S2 option reads:

$$\frac{\Delta C}{\Delta t} = \text{loads} + \text{settling} + \text{production} - \text{resuspension} - \text{losses} - \text{burial} + \text{digging}$$

Resuspension, settling, burial and digging are described in [section 6.6](#). Loss processes are mortality of microphytobenthos, mineralization of detritus fractions, dissolution of opal silicate, desorption of adsorbed phosphate, and degradation of organic micropollutants. Production only applies to the primary production of microphytobenthos.

In the S1-S2 approach all loss processes are essentially described by a zero-order term and a first-order reaction rate:

$$R_{loss} = \frac{k0_{loss}}{H} + \frac{k_{loss} \times Cx}{V}$$

with:

Cx	amount of a substance [gC/N/P/Si]
$k0_{loss}$	zero-order loss rate [g m ⁻² d ⁻¹]
k_{loss}	first-order loss rate [d ⁻¹]
R_{loss}	loss rate [gC/N/P/Si m ⁻³ d ⁻¹]
H	thickness of overlying computational cell [m]
V	volume of overlying computational cell [m ³]

Inorganic nutrients formed by mineralization or desorption are instantaneously released to the overlying water, as the S1-S2 approach does not include pore water. Particulate nutrients can be retained in the sediment through burial. The mineralization of organic matter in the sediment also leads to a sediment oxygen demand. Considering the intentional simplicity of the S1-S2 approach, this module may be applied in cases in which the sediment-water exchange is not a dominant or very dynamic feature.

The mass transport in the sediment for the layered sediment approach is taken care of by an additional process of the Processes Library, described in the additional D-Water Quality user manual 'Sediment Water Interaction'. This process works on the cells of the additional computational grid for the sediment. It considers the advection and dispersion of both particulate and dissolved substances. The advection of particulate substances results from settling (as input) and resuspension (as output). The process converts these fluxes into burial and digging

fluxes across the interfaces of the sediment layers and the lower boundary, depending on fixed porosities. The advection of solutes arises from seepage. Dispersion is described as based on Fick's Law. The dispersion coefficient for particulate substances refers to bioturbation, the dispersion coefficient for solutes to bio-irrigation, flow induced dispersion and diffusion.

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7 Numerical aspects

7.1 Dispersion and turbulent diffusion

Diffusion normally refers to molecular diffusion of gases. In transport equation, the dispersion coefficient stands for all transport that could not be resolved with the finite grid of the Delft3D-FLOW module (Deltares, 2024h). This implies that dispersion is much larger than molecular diffusion. First of all, small scale chaotic movement of water parcels (due to density fluctuations in the water column) will lead to turbulent diffusion. Still this term can be very small. More dispersion enters the modelling effort by small scale eddies that were not resolved on the computational grid. These are the terms that we have to deal with in 3D modelling. Still, in 1D and 2D models diffusion can be much larger and needs serious attention since it can explain much of the mixing processes in the water column. In water quality modelling this term is often referred to as 'dispersion' as it mixes discharged material. To explain turbulent diffusion and the dispersion effect, we will demonstrate it for a small estuary that is treated as a 1-dimensional stretch of elements (the estuary in Figure 7.1). Hereto, we will first derive the 3-dimensional transport equations and then show the effect of limiting the area to 1-dimension.

For the 1-dimensional model we start from the advection-diffusion equation, neglect the reaction terms and source terms, and integrate over y - and z -direction.

$$T_y = \int_{y_l}^{y_r} \frac{\partial}{\partial y} \left(D \frac{\partial C}{\partial y} - v_y C \right) dy = \left(D \frac{\partial C}{\partial y} - v_y C \right) \Big|_{y=y_l}^{y=y_r} = 0 \quad (7.1)$$

with:

$y_r = y$ at right embankment

$y_l = y$ at left embankment

$T_y =$ transport at y

Since no transport along the closed boundaries (the embankments in Figure 7.1) occurs the 'stock terms' at the right hand side of Equation (7.1) vanish.

For the same reason the $\partial/\partial z$ term vanishes after integration over z from bottom to surface. After integrating the 3D advection-diffusion equation over y and z , an equation results with transport for the x -direction only. It is:

$$\frac{\partial}{\partial t}(A\bar{C}) = \frac{\partial}{\partial x} \left(D \frac{\partial A\bar{C}}{\partial x} \right) - \frac{\partial}{\partial x} \int_y \int_z (v_x C) dy dz + A\bar{f}(\bar{C}, \dots, t) + AS \quad (7.2)$$

with:

\bar{C} = average concentration over the cross-section ¹

A = cross-sectional surface

D = molecular diffusion

\bar{f} = cross-sectional averaged water quality processes

S = source terms from discharges

In Equation (7.2) there is one term which will be discussed in more detail here.



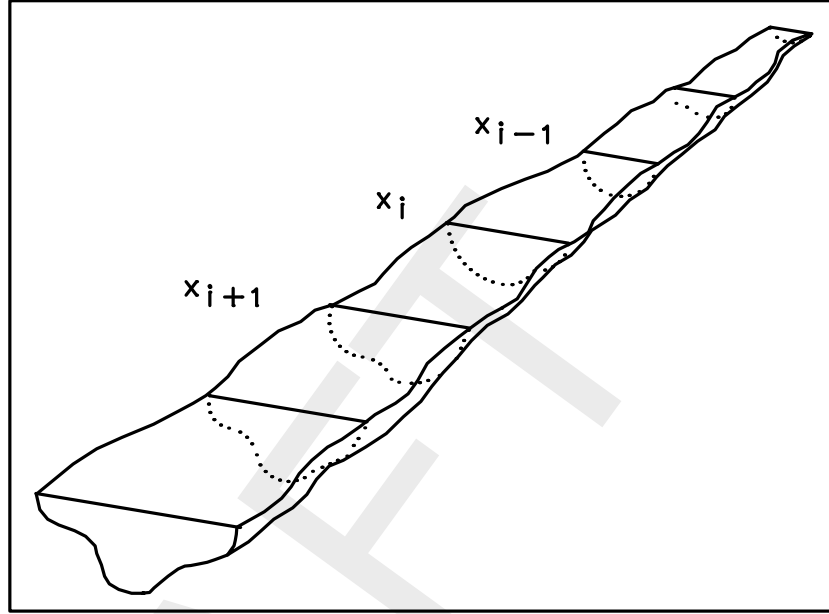


Figure 7.1: Estuary represented as a 1-dimensional model

With:

$$v_x = \bar{v}_x + \Delta v_x \quad \text{and} \quad C_x = \bar{C}_x + \Delta C_x, \quad (7.3)$$

the advective term of Equation (7.2) is:

$$\frac{\partial}{\partial x} \int_y \int_z (v_x C) dy dz = \frac{\partial}{\partial x} (\bar{v}_x \bar{C}_x) + \frac{\partial}{\partial x} \int_y \int_z (\Delta v_x \Delta C_x) dy dz \quad (7.4)$$

If Δv_x and ΔC_x (which are functions of y and z) are not correlated at all, the last term of Equation (7.4) vanishes. However, there are almost always small turbulences in the water. They appear as a positive value of Δv_x at some location and a negative value at neighbouring locations. If the upstream concentration is higher than the downstream concentration, this small turbulence causes an additional positive transport (Figure 7.2).

A well known approximation is, that this transport is proportional to the concentration difference over the small turbulence distance:

$$T_{add} = -\frac{\partial}{\partial x} \int_y \int_z (\Delta v_x \Delta C_x) dy dz \approx -\Delta v_x \Delta x_t \frac{(C_{x+\Delta x_t} - C_x)}{\Delta x_t} \approx -K \frac{\partial C}{\partial x} \quad (7.5)$$

with:

Δx_t = length of the turbulence

K = constant of proportionality ($= \Delta v_x \Delta x_t$)

This formulation is equivalent with the diffusion formulation Equation (7.5) with diffusion of magnitude K . This additional term, which is caused by integrating over the distance of turbulences in space, is called turbulent diffusion. It is generally orders of magnitude higher than the molecular diffusion.

Dispersion

The above given derivation of a turbulent diffusion term K , applies somewhat different if

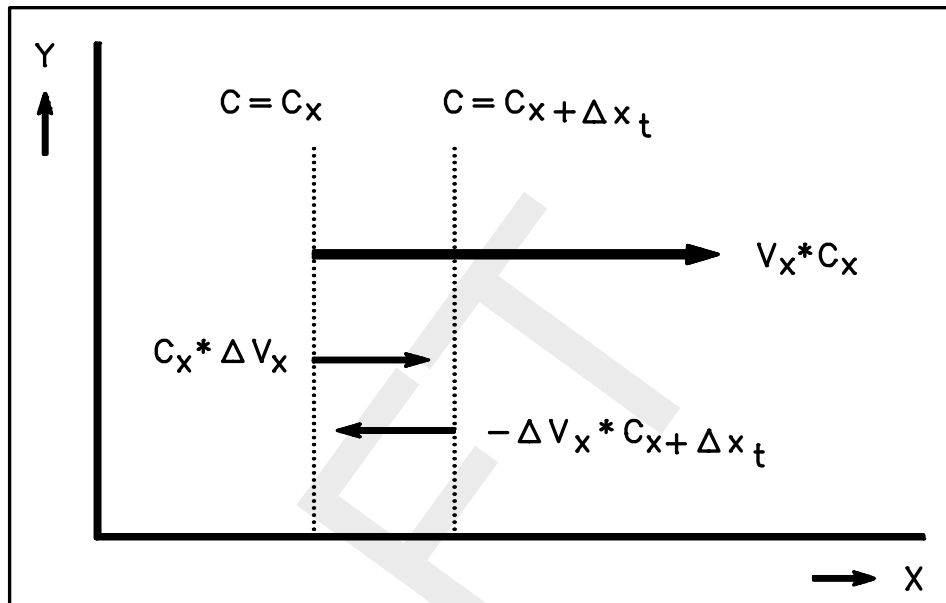


Figure 7.2: Effect of turbulent fluctuations Δv_x on the net transport

integration is performed over the whole cross-sectional area of a small estuary instead of only over the scale of turbulences.

Figure 7.3 shows a one-dimensional estuary with an amount of substance initially distributed uniformly over the cross-section. After a certain amount of time, the substance is not distributed uniformly over the cross-section anymore. Because we integrated in our example over a cross-section however, the resulting cross-sectional average concentration, shows a pattern along the axis of flow, that is very similar to the pattern obtained by a diffusion process. The mixing along a cross-section of the system often takes a much longer time than the time span to generate the picture of Figure 7.3. But the differences over the river width are not distinguished in the one-dimensional model.

The basis of this phenomenon is again the fact that Δv_x and ΔC_x may be correlated and the integral of their product in Equation (7.5) differs from zero. The fact that diffusion type curves result, like in the river example above, is an empirical fact. Only for some well-defined very special situations, a precise computation of the effect can be given. Care must be taken, however.

In e.g. the river situation above, large off-stream parts of the river, called dead zones, cause an asymmetrical shape of the concentration curve along the x -axis, that cannot fully be explained with the one-dimensional advection diffusion equation.

The additional diffusion term, that must account as much as possible for these effects, is often called dispersion. Although experienced modellers have an idea of the magnitude of this term, it is often subject to calibration in models. This term is again orders of magnitude larger than the turbulent diffusion mentioned before.

Dispersion is also much higher than turbulent diffusion used in 3D models. The 3-dimensional models can explain more of the transport in the water column from the hydrodynamics it self and need much less adjustments for unresolved transport. This is not so for the vertical direction since transport by vertical velocities (along the sigma-co-ordinates) can be very small there compared to vertical diffusive transport. Thus, for 3D simulations much attention must still be put into accurate modelling of vertical transport. Using results from accurate turbu-

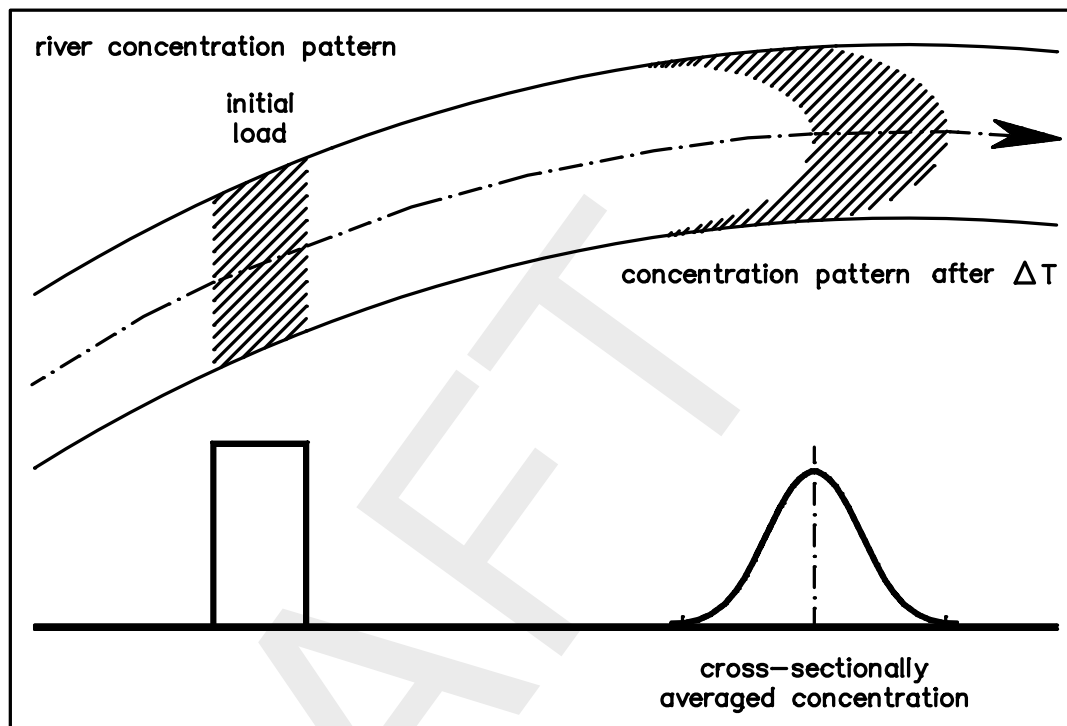


Figure 7.3: "Dispersion" by inhomogeneity of flow in a cross-sectionally averaged one-dimensional model

lence models (incorporated in most if not all hydrodynamic models) is therefore strongly recommended.

The dispersion term of a 2-dimensional horizontal application accounts for depth averaging, but also for horizontal integration over the size of each computational grid cell. If the horizontal grid cells are larger, this horizontal component will become larger. If the horizontal grid cells become smaller, more of the heterogeneity of flow and concentration is explicitly incorporated in the model and consequently the dispersion term becomes smaller. If the horizontal grid cells become very large, then the grid itself mixes so intensively that the dispersion coefficient to be added can be taken smaller, or even has to be set at zero because (initial) mixing is already too large.

Up to now it has been assumed that exact integration over time would take place. Also in time however discrete steps will be taken and the same type of reasoning applies to fast fluctuations lumped in cross terms under the integral. A special situation may exist for tidal areas if a time step of a complete tidal cycle is set and only residual currents are taken into account. In [Table 7.1](#) some common values for molecular diffusion, turbulent diffusion and depth integrated (horizontal) dispersion terms are given. Vertical dispersion is usually orders of magnitude smaller than horizontal dispersion. First of all, this follows from the small length scales in vertical direction. But, small vertical dispersion is found in particular for stratified systems where turbulence is dissipated at a pycnocline by buoyancy forces. This leads to vertical dispersion coefficients of $1.0 \times 10^{-5} \text{ m}^2/\text{s}$. Vertical dispersion is accurately calculated by the turbulence model in Delft3D-FLOW and D-Flow FM.

Table 7.1: Common ranges of horizontal dispersion terms in aggregated models with a finite grid

mixing phenomena	D [m ² /s]
molecular diffusion	1×10^{-9}
vertical diffusion (stratified systems)	$1 \times 10^{-4} - 1 \times 10^{-6}$
vertical diffusion (non-stratified systems)	$1 \times 10^{-1} - 1 \times 10^{-3}$
turbulent diffusion	0.1 – 1.0
depth integration estuaries and seas	10 – 1000
tidal and depth integration estuaries and seas	100 – 1000
one dimensional rivers	100 – 1000

7.2 Introduction to algorithmic implementation

The multi-dimensional water quality program D-Water Quality solves the advection-diffusion-reaction equation. Solution of the advection-diffusion-reaction equation with computers requires the use of discrete segments in space with finite mesh sizes Δx , Δy and Δz and with a finite time-step Δt . Various options for discretising the partial differential equations in terms of Δx , Δy , Δz and Δt are possible. These options are called '*numerical discretisation schemes*'. For example, for the space discretisation *central* discretisations or (first or higher order) *upwind* discretisations may be applied. For the time integration you may choose between *explicit*, *semi-implicit* or *implicit* methods. Having the numerical discretisation different strategies can be followed to solve the discretised systems of equations. These strategies are known as '*solution methods*', and can be divided in *iterative solvers* or *direct solver*. This chapter describes the integration schemes in D-Water Quality for the advection-diffusion-reaction equation. A lot of different integration schemes are available in D-Water Quality. The numerical discretisations and applied iterative solution methods will be described.

Important features of numerical schemes are accuracy (determined by the order of the scheme), robustness (stability and positivity) and efficiency. The choice of the spatial discretisation of the advective terms has great influence on the accuracy, monotonicity and efficiency of the computational method. Central differences are second order accurate, but may give rise to non-physical spurious oscillations, so-called "wiggles" in the solution. These wiggles arise in the vicinity of steep gradients of the quantity to be resolved. On the other hand, first order upwinding is unconditionally wiggle-free or monotone, thus promoting the stability of the solution process, but introduces a truncation error, which has the form of a second-order artificial viscosity term. In advection-dominated flows, this artificial viscosity dominates the physical viscosity and the computed solution is much more smooth than the correct one. Higher order upwinding is not free from numerical oscillations but introduces higher-order artificial viscosity. This higher order viscosity suppresses the wiggles without smoothing the solution too much.

For explicit methods special considerations for the size of the time step must be taken into account (*stability criteria*) in order to get results at all. With respect to 3-dimensional models, special considerations for stability in vertical direction are required. Some discretisations guarantee positive results. Some schemes may lead to spurious oscillations in the concentrations

(although such results may be accurate), and this can make you feel uneasy. Monotonous or TVD (Total Variation Diminishing) results are usually required. Therefore, *positivity* and *monotonicity* are important items for numerical schemes in water quality modelling. Items of accuracy, efficiency, and robustness of the various schemes in D-Water Quality will be addressed in this chapter.

7.3 Conceptual description

7.3.1 Partial differential equations

The advection-diffusion-reaction equation in D-Water Quality reads:

$$\frac{\partial C}{\partial t} = -\vec{u} \cdot \vec{\nabla} C + \vec{\nabla} \cdot \left(\vec{D} \cdot \vec{\nabla} C \right) + S + f_R(c, t) \quad (7.6)$$

where:

$\vec{u} = (u_x, u_y, u_z)$ = flow velocity

$\vec{\nabla} C = \left(\frac{\partial C}{\partial x}, \frac{\partial C}{\partial y}, \frac{\partial C}{\partial z} \right)$ = concentration gradient

$\vec{D} = \begin{pmatrix} D_{xx} & D_{yx} & D_{zx} \\ D_{xy} & D_{yy} & D_{zy} \\ D_{xz} & D_{zy} & D_{zz} \end{pmatrix}$ = diffusion tensor

$\vec{a} \cdot \vec{b}$ = vector dot-product from vector \vec{a} and \vec{b}

$\vec{A} \cdot \vec{b}$ = matrix-vector product from tensor \vec{A} and vector \vec{b}

S = sources and sinks

$f_R(c, t)$ = biological, bacteriological, ecological, chemical or other reactions

An example of a bacteriological reaction is the following first order decay reaction:

$$f_r(c, t) = -kc \quad (7.7)$$

For incompressible flow the conservation law of mass, also known as volume balance, is given by:

$$\vec{\nabla} u = 0 \quad (7.8)$$

The volume balance is computed by Delft3D-FLOW or D-Flow FM, which are Deltares programs for the simulation of non-steady flow and transport phenomena resulting from tidal and meteorological forcing. We remark that in its discretised form care must be taken that the equation is exactly solved. Flow fields should satisfy the volume balance.

7.3.2 Differential equations for computational cells

The finite volume method solves the transport (and reactions) of water and other substances with computational cells. Exact equation (without any discretisation) can be obtained for flux transport between these cells. These equations are derived by integrating Equation (7.6) over the computational cells, and subsequently applying Gauss' divergence theorem:

Gauss' theorem:

$$\int_V \vec{\nabla} \cdot \vec{W} dV = \oint_A \vec{W} \cdot \vec{n} dA \quad (7.9)$$

with \vec{W} an arbitrary vector. The resulting equations are the following integro-differential equations:

ADVECTION-DIFFUSION IN FLUX-FORM:

$$\frac{dM}{dt} + \oint_A (\vec{u}C) \cdot \vec{n} dA = \oint_A (\vec{D} \cdot \vec{\nabla} C) \cdot \vec{n} dA \quad (7.10)$$

CONTINUITY EQUATION:

$$\frac{dV}{dt} + \oint_A \vec{u} \cdot \vec{n} dA = 0 \quad (7.11)$$

with

- M = mass of the substance in the cell
- V = volume
- A = face of the volume
- dA = infinitesimal face element
- \vec{n} = unit vector normal to an infinitesimal face element dA
- \vec{u} = flow velocity

These integro-differential equations are still exact, but contain less detail than the partial differential equations. Concentrations inside the cells are no longer used (only concentrations at the cell face, and concentrations gradients need to be known). By volume averaging also some geometrical information is lost (only the shape of the cell face and its links to its neighbours matters).

The average concentration in a computational cell is given by:

$$\bar{C} = \frac{M}{V} \quad (7.12)$$

with:

- \bar{C} = average concentration in a cell
- M = mass in a cell
- V = volume of a cell

Thus, it is assumed that the average concentration value in a segment is representative of the concentration in the whole volume.

The face integrals represent mass fluxes between the segments. Hydrodynamic packages only compute the flow of water through a cell face, they do not give a detailed description of velocities for small face elements. Therefore, we introduce the flow rate in the transport equation:

$$\oint_A (\vec{u}C) \cdot \vec{n} dA = \sum_{j=1,n} \int_{A_{i \rightarrow j}} (\vec{u}C) \cdot \vec{n} dA \approx \sum_{j=1,n} (Q \cdot \tilde{C})_{i \rightarrow j} \quad (7.13)$$

with:

$$Q_{i \rightarrow j} = \int_{A_{i \rightarrow j}} (\vec{u} \cdot \vec{n}) dA = \text{flow rate}$$

$$\tilde{C} = \frac{\int_{A_{i \rightarrow j}} C dA}{A_{i \rightarrow j}} = \text{cell face averaged concentration}$$

with n the number of neighbouring cells. The pointer index represents the exchanges between volumes i and j . A similar flux equation for diffusion fluxes can be given. The resulting volume averaged equation reads:

$$\frac{d(V\bar{C})_i}{dt} + \sum_{j=1,n} (Q\tilde{C})_{i \rightarrow j} = \sum_{j=1,n} \left(D \frac{\partial \tilde{C}}{\partial x} \right)_{i \rightarrow j} A_{i \rightarrow j} \quad (7.14)$$

Flows and volumes in this equation follow from the hydrodynamic model, possibly via a dedicated coupling module. Also exchange faces A can be derived from the hydrodynamic model. To solve the equation for C and \tilde{C} it is useful to express \tilde{C} in \bar{C} . This is what is done in the various numerical schemes. The resulting continuity equation that follows from Gauss theorem is:

$$\frac{dV_i}{dt} = \sum_{j=1,n} Q_{i \rightarrow j} \quad (7.15)$$

This equation can also be derived by substituting a constant number (constant water density) for concentrations in [Equation \(7.13\)](#).

7.4 Numerical discretisation

7.4.1 Introduction

Important features of numerical schemes are accuracy (determined by the order of the scheme), robustness (stability and positivity) and efficiency. All numerical schemes can be derived from the basic equation:

$$\frac{d(V\bar{C})_i}{dt} = - \sum_{j=1,n} (Q\tilde{C})_{i \rightarrow j} + \sum_{j=1,n} \left(D \frac{\partial \tilde{C}}{\partial x} \right)_{i \rightarrow j} A_{i \rightarrow j} + f_R(\bar{C}_i, t) + S_i \quad (7.16)$$

with:

\bar{C} = average concentration in a cell;

\tilde{C} = face averaged concentration;

V = volume of a cell;

Q = flow through the face of a cell;

A = face area of a cell

D = diffusion coefficient at the face of a cell;

$\frac{\partial \tilde{C}}{\partial x}$ = concentration gradient at the face of a cell;

$f_R(\bar{C}_i, t)$ = mass derivatives for reactions, as a function of concentrations and time;

S = source or sink terms

n = number of neighbouring cells

7.4.2 Time discretisation and stability criteria

Time-discretisation is explicit, implicit or semi-implicit. Consider the equation in form:

$$\frac{\partial c}{\partial t} = Lc \quad (7.17)$$

with:

L = differential operator

The general recipe for time-discretisation for D-Water Quality is:

$$\frac{c^{t+\Delta t} - c^t}{\Delta t} + \text{H.O.T.} = (1 - \theta)(Lc)^t + \theta(Lc)^{t+\Delta t} \quad (7.18)$$

with the time-splitting factor θ :

- 1 $\theta = 0.0$ explicit scheme (Euler's explicit rule)
- 2 $\theta = 1.0$ fully implicit scheme (Euler's implicit rule)
- 3 $\theta = 0.5$ semi-implicit scheme (Trapezoidal rule)

Here H.O.T. stands for Higher-Order-Terms. Some schemes in D-Water Quality expand the time-derivative at the right hand side to second order. Third order terms are not (yet) included in D-Water Quality schemes. The importance of the θ -factor is that schemes with $\theta \geq 0.5$ are *unconditionally stable (robustness)*. For schemes with $\theta < 0.5$ numerical stability is not always guaranteed. Here, stability criteria should be satisfied. If these criteria are not satisfied, small round off errors could amplify quickly and completely erroneous results occur (including overflow). Another robustness factor is positivity. Without any special measures (e.g. filtering) only schemes with $\theta = 0.0$ or $\theta = 1.0$ are positive definite (accuracy and robustness). Schemes with $\theta = 0.5$ (exactly) are unconditionally stable but suffer from serious oscillations and negative results. Therefore, such schemes are not very popular in water quality modelling, although they may be computationally efficient (ADI) and accurate.

Numerical stability conditions

For all explicit schemes ($\theta = 0.0$) in D-Water Quality the 'Courant-Friedrichs-Lewy' (CFL) condition for stability is:

$$\Delta t < \frac{V_i}{\sum_{j=1,n} Q_{i \rightarrow j}} \quad (7.19)$$

This criteria must be satisfied for all computational cells simultaneously. This means in words that:

"The volume of water replaced within any grid cell within one time step must always be smaller than the volume of the grid cell"

Stability criteria can also be derived for the dispersion term:

$$\Delta t < \frac{1}{\left(\frac{2 \sum D_{xx} (A_{yzi \rightarrow j} / V_i)}{\Delta x_i} + \frac{2 \sum D_{yy} (A_{xzi \rightarrow j} / V_i)}{\Delta y_i} + \frac{2 \sum D_{zz} (A_{xyi \rightarrow j} / V_i)}{\Delta z_i} + \frac{\sum_i Q_{i \rightarrow j}}{V_i} \right)} \quad (7.20)$$

From this formula, it can be seen why stability might be a problem in 3D calculations. The term containing the vertical dispersion can get very large, due to the small mesh sizes in

vertical direction, which will be very large for shallow waters. Thus for 3D-problems, nearly always implicit factors are required in vertical direction. D-Water Quality has such schemes. In D-Water Quality it is also possible to use different numerical schemes (with different θ 's) in horizontal and vertical direction.

Time discretisation of reaction terms and source terms

Reaction terms and source terms are always treated explicitly in D-Water Quality. This allows for complex and non-linear reactions, but sometimes instabilities may occur. Since usually the stability criteria for transport is much more stringent this is in practice not a problem. Reaction terms are calculated every time-step. Reaction terms are treated simply with a first order discretisation (no H.O.T.), except for the 2nd order Runge Kutta explicit scheme (Scheme 2).

There are a few exceptions to this rule:

- 1 Intakes from power plants where the rate of intake is "large", that is the volume of water being taken in per time step is comparable or even larger than the volume of the grid cell in which the intake is located.
In this situation the general explicit method for evaluating waste loads (which includes such intakes) implies a limit to the time step. Roughly speaking: the volume taken in per timestep (so rate time time step size) should not exceed the volume of the cell.
- 2 Waste loads as function of time where the time scale of variation is comparable or even shorter than a computational time step. As the waste loads are only evaluated at times that are multiples of the time, it is possible to miss important information. For instance, consider the following time series:

Time [hh:mm]	Value
0:00	0.0
0:01	1000.0
0:02	0.0
1:00	0.0
1:01	1000.0
1:02	0.0
2:00	0.0
2:01	1000.0
2:02	0.0
...	...

which is interpreted as a block function (so between 0:01 and 0:02 the value is constantly 1 000.0). If the time step is 5 minutes, then this function is evaluated at 0:00, 0:05, 0:10 etc. In other words: it will be constantly zero, whereas if the time step were 1 minute, it would be 1 000.0 at 0:01, 0 at 0:02, and so on, precisely as intended.



Note: this is true for all timeseries within D-Water Quality, so one must take care if the time step of the computation is not short vis-a-vis the time scales of the input.

7.4.3 Discretisation of transport and numerical diffusion

This section explains the numerical schemes of D-Water Quality. D-Water Quality calculates mass derivatives (in time) of:

- 1 advective transport
- 2 diffusive transport
- 3 reaction terms
- 4 source terms

D-Water Quality uses the following scheme in order to proceed one step in time:

$$\Delta M_i^{t+\Delta t} = \Delta M_i^t + \Delta t \left(\frac{\Delta M}{\Delta t} \right)_{Tr} + \Delta t \left(\frac{\Delta M}{\Delta t} \right)_R + \Delta t \left(\frac{\Delta M}{\Delta t} \right)_S \quad (7.21)$$

$$C_i^{t+\Delta t} = \frac{M_i^{t+\Delta t}}{V_i^{t+\Delta t}} \quad (7.22)$$

$$\begin{aligned} \left(\frac{\Delta M}{\Delta t} \right)_{Tr} &= \text{mass derivative of advective and diffusive transport} \\ \left(\frac{\Delta M}{\Delta t} \right)_R &= \text{mass derivative of reactions} \\ \left(\frac{\Delta M}{\Delta t} \right)_S &= \text{mass derivative of sources} \end{aligned}$$

All numerical schemes in D-Water Quality (except for scheme 2) use explicit first order schemes for reaction terms and source terms. The derivatives of mass for these terms are just added to the derivative obtained for transport.

It is important to realize yourself that the contribution of the extra processes to the model equations is solved numerically through an *explicit integration in time*:

$$C^{t+\Delta t} = C^t + \Delta t \left(\frac{\partial C}{\partial t} \right)_t \quad (7.23)$$

and

$$\left(\frac{\partial C}{\partial t} \right)_t = f(C^t, FF^t, MP) \quad (7.24)$$

where:

t	time [s]
Δt	time step [s]
C	concentration [g/m ³]
FF	forcing function[s]
MP	model parameters

The new concentration value is computed starting from the old value, using the derivative of time which is multiplied with the time step. The derivative of time is computed using the concentrations and forcing functions at the *old time level*. Such a solution technique is characterized by a stability limit to the time step: if the time step is too large compared to the speed of the processes involved, the computation becomes unstable or inaccurate. For a process with a time constant k [1/d], a guideline to obtain a stable and accurate solution would be:

$$\Delta t < \frac{1}{2|k|} \quad (7.25)$$

Thus, the quicker the process (higher value of k), the smaller the allowed time step.

For dispersive transport, concentration gradients in D-Water Quality always follow from a *central discretisation*:

$$\frac{\partial \tilde{C}}{\partial x} \approx \frac{\bar{C}_j - \bar{C}_i}{\Delta x_{i \rightarrow j}} \quad (7.26)$$

with C_i and C_j concentrations on either side of the face between segments i and j .

The remainder of this section deals with mass derivatives of advective transport.

The basic flux-equation (mass flux) for D-Water Quality, with centrally discretised gradients for diffusion, and with a θ -splitting in time is:

$$\begin{aligned} \frac{M_i^{t+\Delta t} - M_i^t}{\Delta t} + \dots \text{(H.O.T.)} = (1 - \theta) \left[- \sum_{j=1,n} (Q\tilde{C})_{i \rightarrow j} + \sum_{j=1,n} D_{i \rightarrow j} \frac{\bar{C}_j - \bar{C}_i}{\Delta x} A_{i \rightarrow j} \right]^t \\ + (\theta) \left[- \sum_{j=1,n} (Q\tilde{C})_{i \rightarrow j} + \sum_{j=1,n} D_{i \rightarrow j} \frac{\bar{C}_j - \bar{C}_i}{\Delta x} A_{i \rightarrow j} \right]^{t+\Delta t} + \left(\frac{\Delta M}{\Delta t} \right)_R^t + \left(\frac{\Delta M}{\Delta t} \right)_S^t \end{aligned} \quad (7.27)$$

The schemes of D-Water Quality now differ in the choice for the implicitness of the time integration (θ), the choice for the face averaged concentration \tilde{C} and the number of H.O.T. that are used to estimate higher order derivatives in time. For some schemes corrections are used to damp spurious oscillations. These corrections are not incorporated in this equation, but will be described for the specific schemes.

7.5 Numerical schemes in D-Water Quality

First, we will summarise the numerical schemes in D-Water Quality briefly. The subsequent sections provide detailed information for each numerical scheme.

Note: A number of schemes have been removed, which explains the "holes" in the numbering. These schemes were not used for a long time, because they could only be applied in special situations or are simply not fit for current practice, like large three-dimensional schematisations.

Overview of numerical schemes in D-Water Quality

Numerical schemes

◇ Schemes 1 and 5:

- Explicit (stability criterion!)
- In practice only applied in 2D simulations as the vertical direction usually results in a very small time step (notably the influence of dispersion)
- scheme 1 is most robust
- scheme 5 is most accurate (2^{nd} order scheme)
- (schemes 2 to 4 have been removed, as they were suitable only for special cases and more general schemes are available)

◇ Schemes 11 to 14:

- Separate solution of horizontal and vertical transport
- Horizontal transport explicit either according to scheme 1 or scheme 5 (stability criterion!)
- Vertical transport implicit
- Central or Upwind discretisation in the vertical
- Upwind schemes may cause numerical mixing which is undesirable when a significant vertical gradient exists
- Scheme 12 (in horizontal as scheme 5 (thus most accurate), in vertical central) is preferred
- ◇ Schemes 15 and 16:
 - Implicit (both in the vertical and in the horizontal)
 - Iterative solvers of the matrix (may be time efficient)
 - Upwind (scheme 15) and Central (scheme 16) in the vertical
 - Numerical mixing of steep gradients occurs
- ◇ (Schemes 19 and 20 have been removed, as they were applicable only to structured grids)
- ◇ Scheme 21 and 22:
 - Improvement on the flux-corrected transport scheme (scheme 5)
 - Avoids the introduction of local extrema by switching between a local explicit and implicit solution method
 - Scheme 21 uses the flux limiter of Salezac, while scheme 22 uses the flux limiter of Boris and Book
- ◇ Scheme 23:
 - Experimental implementation of the QUICKEST scheme
 - Should only be used for two-dimensional models, as it does not currently provide adequate handling for the vertical (third) dimension.
- ◇ Scheme 24:
 - Improvement on the flux-corrected transport scheme (scheme 5)
 - Solves the general stability problem by applying a local time step reduction and can therefore be used with large time steps – generally the same step as the hydrodynamic database
 - Solves the stability problems associated with very small volumes and rapid changes in volume in case of drying and flooding
 - It does have limitations: no additional velocities or dispersions per substance (so some rather specific processes are incompatible with this scheme). Only for the vertical direction this is allowed
 - It is known that the option "no dispersion if the flow rate is zero" must be switched on. If not, the scheme may produce so-called not-a-numbers and these will propagate throughout the model area.
 - If you use this scheme, set the horizontal dispersion coefficient to zero, otherwise the calculation for many segments may require very short time steps and that causes the calculation to become very slow. When the grid is fine enough and a three-dimensional model is used, horizontal dispersion has little or no effect anyway.
 - More detailed documentation is available, which includes a description of several parameters for use with this scheme

Considerations for choice of numerical schemes

- ◇ Accuracy:

- decreases with time step (due to numerical dispersion)
- upwind schemes have numerical dispersion
- central schemes may produce negative concentrations
- implicit schemes smooth gradients
- ◇ Stability:
 - explicit schemes require smaller time steps
- ◇ Positivity:
 - some schemes may produce negative concentrations
- ◇ Efficiency:
 - smaller time step → longer computation time
 - aggregation not always possible
 - convergence of solver

Rule of thumb choice of numerical scheme

1. Scheme 15/16 → Generally very fast scheme, but numerical dispersion may be large
2. Scheme 21/22/24 → fast but accuracy dependent on time step, no stability criterion
3. Scheme 12 (3D) or scheme 5 (2D) → accurate, but must fulfil stability criterion
- 4a. Scheme 1 → less accurate than scheme 5, but more robust (larger time step)
- 4b. Scheme 10 → only 2D, less accurate than scheme 5, but no stability criterion

7.5.1 Upwind scheme (Scheme 1)

This scheme uses $\theta = 0$ (explicit) for time. There are no H.O.T. for time discretisation. The face concentration \tilde{C} is discretised as follows:

$$\tilde{C}_{i \rightarrow j} = \begin{cases} \bar{C}_i & \text{for } Q_{i \rightarrow j} > 0 \\ \bar{C}_j & \text{for } Q_{i \rightarrow j} < 0 \end{cases} \quad (7.28)$$

For the segment adjacent to the cross-section, the concentration is used from one segment only. This is the segment where the flows comes from (or *backward* in space). Since usually the flow comes from the direction where the wind comes from, this method is called '*upwind discretisation*'.

The discretised equation for scheme 1 reads:

$$\begin{aligned} \frac{M_i^{t+\Delta t} - M_i^t}{\Delta t} = & \left[- \sum_{j=1,n}^{\text{outflowing}} Q_{i \rightarrow j} \bar{C}_i - \sum_{j=1,n}^{\text{inflowing}} Q_{i \rightarrow j} \bar{C}_j + \sum_{j=1,n} D_{i \rightarrow j} \frac{(\bar{C}_j - \bar{C}_i)}{\Delta x} A_{i \rightarrow j} \right]^t \\ & + \left(\frac{\Delta M}{\Delta t} \right)_R^t + \left(\frac{\Delta M}{\Delta t} \right)_S^t \end{aligned} \quad (7.29)$$

The method is:

- ◇ computationally very efficient if stability criteria can be met easily (for cells with large residence times, see below). This is not the case for most 3D problems.
- ◇ positive
- ◇ conditionally stable, according to the CFL condition.

- ◇ first order accurate, the second order error is known as *numerical dispersion* and can be *estimated* with the following formulae:

$$D_{num} = \frac{1}{2}(u\Delta x - u^2\Delta t) \quad (7.30)$$

E.g.: $u = 0.1 \text{ m/s}$, $\Delta x = 1000 \text{ m}$, $\Delta t = 0.5 \text{ h} \Rightarrow D_{num} = 41 \text{ m}^2/\text{s}$

The second order error leads to inaccurate description of steep concentration gradients. Therefore, this option is not advised for outfall studies, or studies with 2D/3D-dimensional modelling of sharp concentration fronts (like sediment fronts in coastal zones, salinity fronts etc.).

7.5.2 Second order Runge-Kutta (Scheme 2), Lax Wendroff method (Scheme 3) and Alternating Direction Implicit (2D) method (Scheme 4)

These schemes have been removed.

7.5.3 Flux Correct Transport (FCT) Method (Scheme 5)

This method combines the values of positivity of scheme 1, and accuracy of scheme 3. It works as follows: Scheme 1 is used to get a first estimate of concentrations. Subsequently, the difference between scheme 1, and scheme 3 is calculated. This difference is an anti-diffusion term, and therefore may lead to oscillations. Where diffusion smoothens gradients, anti-diffusion creates gradients.

According to a formula of Boris and Book ([Boris and Book, 1973](#)), anti-diffusion is applied only when for a segment no new minimum and maximum occur (i.e. no oscillations). The condition of Boris and Book uses also the concentrations from neighbouring segments ($i - 1$) and ($j + 1$).

In the coupling to both Delft3D-FLOW and D-Flow FM you have the option to aggregate grids. Irregular aggregated grids might cause this method not to work properly as information on neighbouring grid cells is lost during aggregation.

The anti-diffusion term is a flux term (whether or not it is applied, mass is conserved). Therefore, this method is known as a 'Flux Correct Transport' method. The method is:

- ◇ Accurate to second order if the anti-diffusion term is used throughout (in such a case the method is equivalent to method 3);
- ◇ Accurate to first order if the anti-diffusion term is never applied (in such a case the method is equivalent to method 1);
- ◇ The method is explicit in time. Stability criteria are the same as for method 1 (and 3);
- ◇ The method may artificially damp existing (true) oscillations (e.g. close to sources)
- ◇ The method is positive, *except for errors in the order of machine precision*.
- ◇ computationally very efficient if stability criteria can be met easily (for cells with large residence times, see below). This is not so for most 3D models.

7.5.4 Steady-state solutions (Schemes 6 to 9, 17 and 18)

Not available in D-Water Quality. Their purpose was to determine a steady-state solution, but this approach has inherent limitations and current-day are powerful enough to generate such a solution via a general method.

7.5.5 Implicit Upwind scheme with a direct solver (Scheme 10)

This scheme has been removed, as it is impractical with current-day model schematisations.

7.5.6 Horizontal Upwind scheme, Vertical: implicit in time and central discretisation (Scheme 11)

Method 11 uses a centrally discretised numerical scheme in the vertical direction. Therefore, it need not be positive, and can lead to spurious oscillations, especially in stratified systems.

The method is:

- ◇ computationally very efficient if stability criteria can be met easily for the horizontal direction (for cells with large residence times).
- ◇ not positive. Spurious oscillations and negative concentrations may occur for stratified systems.
- ◇ condition ally stable in the horizontal direction, according to the CFL condition.
- ◇ accurate to second order in vertical direction, but to first order in horizontal direction.

An alternative to this method is scheme 15.

7.5.7 Horizontal: FCT scheme, Vertical: implicit in time and central discretisation (Scheme 12)

This scheme is like scheme 11. However, in horizontal direction scheme 5 (FCT) is applied instead of scheme 1. This leads to higher order accuracy for horizontal directions. Note that results for scheme 12 may look like those for scheme 11 in many applications. Firstly, this will be so for completely unstructured (i.e. irregular aggregated) grids. Secondly, practical experience showed that this is also true for many simulations on structured grids for *stratified* systems or systems with *limited vertical dispersion*.

If the vertical dispersion is large the concentration difference between the layers will disappear and all will be reduced to a 2D problem. If the vertical dispersion is small concentration differences between vertical layers will occur. In such case, the horizontal mixing due to numerical dispersion may be (much) less than the mixing due to exchange between the vertical layers.

The method is:

- ◇ Computationally very efficient if stability criteria can be met easily for the horizontal direction (for cells with large residence times). It less efficient than scheme 11.
- ◇ Not positive. Spurious oscillations and negative concentrations may occur for stratified systems.
- ◇ Condition ally stable in the horizontal direction, according to the CFL condition.
- ◇ Accurate to second order in vertical direction. The accuracy in horizontal direction is in principle second order, but may be first order locally.

7.5.8 Horizontal: Upwind scheme, Vertical: implicit in time and upwind discretisation (Scheme 13)

This scheme is like scheme 11. However, in vertical direction scheme 1 (Upwind) is applied instead of scheme 4. This will lead to lower order accuracy for vertical directions, but positivity will be guaranteed.

The method is:

- ◇ Computationally very efficient if stability criteria can be met easily for the horizontal direction (for cells with large residence times).
- ◇ Positive.
- ◇ Conditionally stable in the horizontal direction, according to the CFL condition.
- ◇ First order accurate in all directions, in vertical direction it is second order accurate in time. *In case of stratified systems, artificial mixing may result between the layers above and below the pycnocline.*

7.5.9 Horizontal: FCT scheme, Vertical: implicit in time and upwind discretisation (Scheme 14)

This scheme is like scheme 12. However, in vertical direction scheme 1 (Upwind) is applied instead of scheme 4. This will lead to lower order accuracy for vertical directions, but positivity will be guaranteed.

The method is:

- ◇ Computationally very efficient if stability criteria can be met easily for the horizontal direction (for cells with large residence times).
- ◇ Positive and monotone.
- ◇ Conditionally stable in the horizontal direction, according to the CFL condition.
- ◇ First order accurate in vertical direction for space discretisation, In vertical direction it is second order accurate in time. The accuracy in horizontal direction is in principle second order, but may locally be first order. *In case of stratified systems, artificial mixing may result between the layers above and below the pycnocline.*

7.5.10 Implicit Upwind scheme with an iterative solver (Scheme 15)

This method deals with *exactly* the same system of linear equations as scheme 10. However, the method to solve these equations is different. The method is an *iterative solver*: it takes a guess for the concentration vector (if available, this guess is the concentration of the previous time-step), and subsequently the method checks if this guess was correct or not. The method is intelligent in such a way, that it will use a next guess that always *must be better* than the previous guess, i.e. the squared sum of differences of all concentrations (the *residual*) will get less. This method is called the Generalised Minimal RESidual method (GMRES) (Saad and Schultz, 1986). *Convergence is always guaranteed.* When the (normalised) residual is small enough (below a *convergence threshold* to be specified by the user), convergence is assumed and the iterative process stops. The convergence threshold is by default 10^{-7} for a normalised residual, but can be adapted by the user. The maximum number of iterations (one iteration is one guess) is 100, but can be adapted also.

Although convergence is guaranteed, still many iterations may be required for convergence. In order to improve the convergence of the method, a pre-conditioner was devised (WL | Delft Hydraulics, 1994, 1996). This implies that the system of equations is transformed to a system that can be solved more easily:

$$M^{-1}A \vec{c} = M^{-1} \vec{b} \quad (7.31)$$

When M is easily inverted the method will not become inefficient (contrary to scheme 10 which is based on an expensive method of matrix inversion). When M resembles A , the method can be expected to converge much faster, since the matrix product $M^{-1} \cdot A$ is nearly the unit matrix. In D-Water Quality a Gauss-Seidel pre-conditioner with two sweeps was used. For the vertical direction a line solver is used, a guess of the solution is made here with a direct method. The advantage of the line solver is that it also converges fast for stratified systems.

In horizontal direction convergence of the method is generally best when the diagonal entries are large. Looking at the diagonal entries given in the formulae of scheme 10 (that is also valid here), this will always be achieved (for all flow conditions) when time-steps are small compared to the water volume of the cell. Thus, *for large time-steps, convergence may be (much) slower than for small time-steps*. It is evident that there is some trade-off for computational efficiency. When making estimates of this trade-off, one must take into account the computer time required for calculating the reaction terms. Contrary to scheme 10, the method is applied to every substance individually. Thus CPU costs are linear with the number of substances. But by taking large time steps the costs of calculating processes may be reduced a lot.

The method is:

- ◇ computationally efficient if large time-steps are used, especially most 3D problems;
- ◇ it may also be used for *unstructured* grids.
- ◇ for simulations with hundreds of substances that all have equal transport the method may get less efficient.
- ◇ positive.
- ◇ there are no stability criteria for Δt for transport. Therefore large time-steps may be used, the size being restricted by accuracy and stability criteria for processes.
- ◇ first order accurate, the second order error is known as *numerical dispersion* (see scheme 1). Numerical dispersion may lead to artificial mixing over the pycnocline in stratified systems.

7.5.11 Implicit Upwind scheme in horizontal, centrally discretised vertically, with an iterative solver (Scheme 16)

This method is like scheme 15, but a centrally discretised scheme is used for the vertical direction. For scheme 15, numerical dispersion may lead to artificial mixing over the pycnocline in stratified systems. Due to the use of the pre-conditioner in scheme 15, there is no objection against the use of centrally discretised systems in vertical direction for this iterative solver (otherwise convergence might be very slow). For stratified systems it may be required to use scheme 16 instead of scheme 15. However, positivity is no longer guaranteed for scheme 16.

The method is:

- ◇ computationally efficient if large time-steps are used, especially most 3D problems;
- ◇ it may also be used for *unstructured* grids;
- ◇ for simulations with hundreds of substances that all have equal transport the method may get less efficient.
- ◇ not strictly positive, nor monotone;
- ◇ there are no stability criteria for Δt for transport. Therefore large time-steps may be used, the size being restricted by accuracy and stability criteria for processes;
- ◇ first order accurate in the horizontal but second order accurate in vertical direction.

7.5.12 ADI scheme for 3D models (horizontal: higher order scheme, vertical: central and upwind discretisation (Schemes 19 and 20))

These schemes have been removed.

7.5.13 Local-theta flux-corrected transport scheme (Scheme 21 and 22)

Scheme 5 in D-Water Quality represents a flux-corrected transport scheme where horizontal transport is first treated using central differences (a second-order method), and if local maxima or minima occur just enough numerical dispersion is added to avoid the occurrence of such extrema. The local-theta method is more or less a refinement of this idea.

The scheme works by solving the equations for a cell with an explicit method first. If the Courant number for the cell is small enough (the CFL-criterium is met), then no further processing is needed. Otherwise an implicit method is used where just enough numerical dispersion is added to avoid local minima or maxima in the complete surroundings of the cell.

Scheme 21 uses the flux limiter of Salezac, while Scheme 22 uses the flux limiter of Boris and Book. The method of Boris and Book looks in the flow direction only to limit the flux correction term. Salezac's method looks around a cell, but that has disadvantages in stratified systems.

For the technical details, see [Slingerland *et al.* \(2009\)](#).

7.5.14 QUICKEST scheme (Scheme 23)

As mentioned in the previous section, this scheme has been implemented only experimentally. In principle it is an accurate scheme, but the current implementation easily leads to instabilities, especially for three-dimensional models. Therefore it should only be used with two-dimensional models (both dimensions horizontal).

The technical details are described in detail in [Nishikawa \(2021\)](#).

7.5.15 Flux-corrected transport with adaptive time-stepping (scheme 24)

The general treatment of the transport equations is the same as for schemes 5 and 12 (flux-corrected transport according to [Boris and Book, 1973](#)) for the horizontal directions and central differences for the vertical direction. However, the time step is adaptive to allow an explicit time integration:

- ◇ The solver uses "baskets" to classify the segments based on the allowed time step. Per time step the solver determines for which segments the given time step can be used without violating the stability criterium. These are listed in basket 1. Segments that require half that step to adhere to the stability criterium are placed in basket 2 and so on.
- ◇ By default 13 baskets are used, so that the smallest time step is 2^{-12} times the given time step (to give a numerical example: if the given time step is one hour, the time step used with the last basket is about 0.88 seconds).
- ◇ Those segments for which even this is too large a time step are treated separately, as are segments that do not participate in the transport ("dry" segments).
- ◇ The details of this classification are printed by turning on the "iteration report" option (for this, define a constant by the name `Iteration report`, note the space). For segments for which the smallest time step is still too large, extra information is given, so that you can examine the stability issues.
- ◇ These "sensitive" segments are treated first and then all the other segments are handled with the time step belonging to the respective baskets.
- ◇ The number of baskets influences the computation time and to some extent the result.

Sometimes it is advantageous to define a smaller number of baskets, so that the computation time is reduced. The solution may then be different by several percent. You can set the number of baskets by defining a constant called `Number_of_baskets` (including the underscores) as part of the process parameters.

- ◇ Note that the classification has to be determined per time step, as the flow field is likely to change over time.
- ◇ By default, the vertical direction is treated using central differences, but you can change this by specifying the option `SCHEME24_VERTICAL_UPWIND` as one of the keywords after the integration option in the input file.
- ◇ A limitation of the scheme is that it does not allow additional velocities or diffusion coefficients per substance. This would require a re-classification of the segments per substance.

However, for vertical transport, for instance the sedimentation of particulate matter, there is no such restriction. It is even possible to select upwind (upstream) differences for the advective component, independent of the general treatment. This is done via the *command-line option* `-settling_backwards`.

7.6 Artificial vertical mixing due to σ co-ordinates

When the FLOW model used the σ -grid in the vertical, then the WAQ model also uses this grid in the vertical. The sigma transformation is boundary-fitted in the vertical. The bottom boundary and free surface are represented smoothly. The water column is divided into the same number of layers independent of the water depth. In a σ -grid, the vertical resolution increases automatically in shallow areas.

For steep bottom slopes combined with vertical stratification, sigma transformed grids introduce numerical problems for the accurate approximation of horizontal gradients in the horizontal diffusion term. Due to truncation errors artificial vertical mixing may occur, (Leendertse, 1990; Stelling and Van Kester, 1994). This artificial vertical transport is sometimes called “creep”.

Let ζ be the position of the free surface, d the depth measured downward positive and H the total water depth. The transformation from Cartesian co-ordinates to σ co-ordinates is defined by:

$$x = x^*, y = y^*, \sigma = \frac{z - \zeta}{H} \quad (7.32)$$

For the horizontal diffusion term, the transformation from Cartesian co-ordinates to σ co-ordinates leads to various cross derivatives. For example, the transformation of a simple second order derivative leads to:

$$\frac{\partial^2 c}{\partial x^2} = \frac{\partial^2 c^*}{\partial x^{*2}} + \left(\frac{\partial \sigma}{\partial x} \right)^2 - \frac{\partial^2 c^*}{\partial \sigma^2} + 2 \frac{\partial \sigma}{\partial x} - \frac{\partial^2 c^*}{\partial x^* \partial \sigma} + \frac{\partial^2 \sigma}{\partial x^2} - \frac{\partial c^*}{\partial \sigma}. \quad (7.33)$$

For such a combination of terms it is difficult to find a numerical approximation that is stable and positive, see (Huang and Spaulding, 1996). Near steep bottom slopes or near tidal flats where the total depth becomes very small, truncations errors in the approximation of the horizontal diffusive fluxes in σ co-ordinates are likely to become very large, similar to the horizontal pressure gradient.

Following Delft3D-FLOW the tensor is redefined in the σ co-ordinate system assuming that the horizontal length scale is much larger than the water depth (Blumberg and Mellor, 1987)

and that the flow is of boundary-layer type. The horizontal gradients are taken along σ - planes. This approach guarantees a positive definite operator, also on the numerical grid (Beckers *et al.*, 1998). For a detailed description we refer to Chapter 9 of the FLOW User Manual (Deltares, 2024h).

If the same approach is used for the horizontal diffusion operator in the transport equation:

$$\frac{\partial^2 c}{\partial x^2} \approx \frac{\partial^2 c^*}{\partial x^{*2}}, \quad (7.34)$$

Horizontal diffusion will lead to vertical transport of matter through vertical stratification interfaces (pycnocline) which is unphysical. A more accurate, strict horizontal discretization is needed.

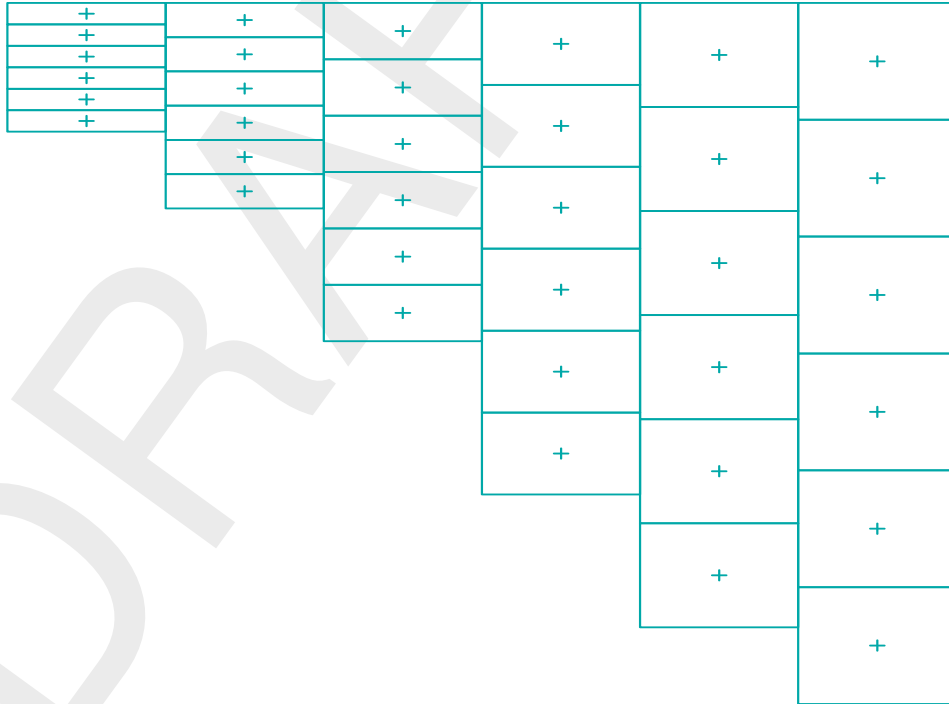


Figure 7.4: Finite Volume for diffusive fluxes and pressure gradients

Like in Delft3D-FLOW, in D-Water Quality an option is available that minimises artificial vertical diffusion due to truncation errors; see ???. A method has been implemented which gives a consistent, stable and monotonic approximation of the horizontal diffusion term. This “anti-creep” option is based upon a Finite Volume approach; see Figure 7.4. The horizontal diffusive fluxes and baroclinic pressure gradients are approximated in Cartesian co-ordinates by defining rectangular finite volumes around the sigma co-ordinate grid points. Since these boxes are not nicely connected to each other, see Figure 7.5, an interpolation in z -co-ordinates is required to compute the fluxes at the interfaces.

Since the centres of the finite volumes on the left-hand side and right-hand side of a vertical interval are not at the same vertical level, a z -interpolation of the scalar concentration c is needed to compute strictly horizontal derivatives. The values obtained from this interpolation are indicated by c_1^* and c_2^* respectively in Figure 7.5. Stelling and Van Kester (1994) apply a non-linear filter to combine the two consistent approximations of the horizontal gradient,

$$s_1 = \frac{c_2^* - c_1}{\Delta x} \text{ and } s_2 = \frac{c_2 - c_1^*}{\Delta x}:$$

If $s_1 \times s_2 < 0$ Then

$$\frac{\Delta c}{\Delta x} = 0$$

Else

$$\frac{\Delta c}{\Delta x} = \text{sign}(s_1) \times \min(|s_1|, |s_2|)$$

Endif

(7.35)

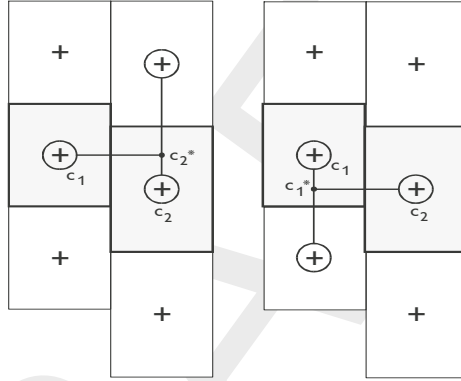


Figure 7.5: Left and right approximation of a strict horizontal gradient

If an interval has only grid boxes at one side, the derivative is directly set to zero. The horizontal fluxes are summed for each control volume to compute the diffusive transport. The integration of the horizontal diffusion term is explicit with time step limitation:

$$\Delta t \leq \frac{1}{D_H} \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right)^{-1}. \quad (7.36)$$

Since this approximation of the horizontal gradient is used for the horizontal diffusion flux, it is important to ensure that the difference operator is positive definite in order to get physically realistic solutions. The maximum and minimum of a variable being transported by diffusion do not increase or decrease (min-max principle). By taking the minimum of the gradients, [Stelling and Van Kester \(1994\)](#) show that, the min-max principle is fulfilled. [Beckers et al. \(1998\)](#) show that any nine-point consistent linear discretization of the horizontal diffusion on the σ -grid does not fulfil the min-max principle. From numerical tests [Slørdal \(1997\)](#) concluded that the underestimation is reduced by increasing the vertical resolution, but is sometimes enhanced by increasing the horizontal resolution.

Let s_4 be a consistent approximation of the horizontal gradient $s_4 = \frac{s_1 + s_2}{2}$. [Slørdal \(1997\)](#) suggested to take s_4 as approximation of the horizontal gradient. He calls his approach the “modified Stelling and Van Kester scheme”. It is equivalent to linear interpolation at a certain z -level before taking the gradient. It is more accurate than taking the minimum of the absolute value of the two slopes s_1 and s_2 but it does not fulfil the min-max principle for the diffusion operator. It may introduce wiggles and a small persistent artificial vertical diffusion. Due to the related artificial mixing, stratification may disappear entirely for long term simulations, unless the flow is dominated by the open boundary conditions.

By introducing an additional approximation of the horizontal gradient in the filter algorithm defined by $s_3 = \frac{c_2 - c_1}{\Delta x}$, the stringent conditions of the minimum operator can be relaxed somewhat. This third gradient s_3 , which is consistent for $\min(|s_1|, |s_2|) < s_3 < \max(|s_1|, |s_2|)$,

has point-to-point transfer properties and therefore leads to a positive scheme for sufficiently small time steps. The following non-linear approach presently available in D-Water Quality is both consistent and assures the min-max principle:

$$\begin{aligned}
 &\text{If } s_1 \times s_2 < 0 \quad \text{Then} \\
 &\quad \frac{\Delta c}{\Delta x} = 0 \\
 &\text{Elseif } |s_4| < |s_3| \quad \text{Then} \\
 &\quad \frac{\Delta c}{\Delta x} = s_4 \\
 &\text{Elseif } \min(|s_1|, |s_2|) < |s_3| < \max(|s_1|, |s_2|) \quad \text{Then} \\
 &\quad \frac{\Delta c}{\Delta x} = s_3 \\
 &\text{Else} \\
 &\quad \frac{\Delta c}{\Delta x} = \text{sign}(s_1) \min(|s_1|, |s_2|) \\
 &\text{Endif}
 \end{aligned} \tag{7.37}$$

The method requires a binary search to find the indices of neighbouring grid boxes, which is time consuming. The increase in computation time is about 30%.

If the streamlines are strictly horizontal, transport of matter discretised on a σ -co-ordinate grid may still generate some numerical vertical diffusion by the discretization of the advection terms.

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A File descriptions

A.1 Overview of files

Within the process of the setting up a water quality simulation many files are generated and many files may be used. [Table A.1](#) contains an overview of the files used in some way in D-Water Quality.

Table A.1: Files in D-Water Quality

File extension	Description	Output from	Input for
*.0	Configuration file for the Processes Library Configuration Tool (PLCT)	PLCT	PLCT
.ada	Result file with spatial information in NEFIS format. Always accompanied by <.adf> file	WAQ(2)	GPP
.adf	NEFIS definition file of <.ada> file	WAQ(2)	GPP
*.are	Model schematisation file containing the exchange areas between computational cells in [m ²]	hydrodynamic model	WAQ(2)
*.atr	Model schematisation file containing the attributes of the computational cells. Attributes indicate the vertical position of the computational cell: 0 = surface and bottom layer (z-layer or 2D simulation) 1 = surface layer 2 = intermediate layer 3 = bottom layer	hydrodynamic model	WAQ(2)
*-bal.his	Result file with mass balances per observation point for each substance	WAQ(2)	GPP
*.chz	Model schematisation file containing Chézy values of the computational cells	hydrodynamic model	–
*.dwq	Horizontal aggregation file	DIDO	hydrodynamic model
*.flo	Model schematisation file containing the flows between computational cells in [m ³ /s]	hydrodynamic model	WAQ
.hda	Result file with time-series information at observation points in NEFIS format. Always accompanied by <.hdf> file	WAQ(2)	GPP
.hdf	NEFIS definition file of <.hda> file	WAQ(2)	GPP
continued on next page			

Table A.1 – continued from previous page

File extension	Description	Output from	Input for
*.his	Result file with time-series information at observation points in binary format	WAQ(2)	GPP
*.hyd	Coupled hydrodynamics information file	hydrodynamic model	D-Water Quality
*.inc	Include files, parts of the .inp file that are written by D-Water Quality	D-Water Quality	WAQ(1)
*.inp	Input file for water quality simulation	D-Water Quality	WAQ(2)
*.len	Model schematisation file containing the dispersion lengths of computational cells in [m]	hydrodynamic model	WAQ(2)
*.lsp	Report file of the pre-processor for a water quality simulation containing information on which water quality processes are selected (switched on) and the determination of where to retrieve the parameter input for the processes	WAQ(1)	–
*.lst	Report file of the pre-processor for a water quality simulation containing the check on the correctness of the input	WAQ(1)	–
*.map	Result file with spatial information in binary format	WAQ(2)	GPP
_res.map	Restart file in <.map> format containing the concentration of each substance after the last computational time step	WAQ(2)	D-Water Quality GPP
*-stat.map	Result file with spatial information of statistical output	WAQ(2)	GPP
*.mon	Result file with time-series information and (total) mass balance information at observation points in ASCII format. Also contains error messages that occur during a water quality simulation.	WAQ(2)	–
*-stat.mon	Result file with statistical information at observation points in ASCII format	WAQ(2)	–
*.poi	Model schematisation file containing the linkages (pointers) between the computational cells	hydrodynamic model	WAQ(2)
continued on next page			

Table A.1 – continued from previous page

File extension	Description	Output from	Input for
*_res.map	Restart file containing the concentration of each substance after the last computational time step	WAQ(2)	WAQ(1)
.sal	Salinity values in [g/kg] derived from the hydrodynamic simulation through the <com-.dat> file	hydrodynamic model	–
*.srf	Model schematisation file containing the horizontal surface areas of the computational cells in [m ²]	FM	WAQ
*.stt	Input file for specifying statistical output for a water quality simulation	- WAQ(1)	–
*.sub	Substances file containing the state variables (substances), processes, editable input parameters and output parameters to be included in the water quality simulation	PLCT	D-Water Quality
.tau	Shear stress values (Tau) in [N/m ²] derived from the hydrodynamic simulation through the <com-.dat> file	hydrodynamic model	–
.tem	Water temperature values in [°C] derived from the hydrodynamic simulation through the <com-.dat> file	hydrodynamic model	–
*.vol	Model schematisation file containing the volumes of the computational cells in [m ³]	hydrodynamic model	WAQ(2)
*.wrk	Temporary work files containing the pre-processed information for the water quality simulation	WAQ(1)	WAQ(2)
.vdf	Vertical dispersion values in [m ² /s] derived from the hydrodynamic simulation through the <com-.dat> file	hydrodynamic model	WAQ(2)
*.wlk	Model schematisation file containing information on so-called walking discharges. Walking discharges can change their position if the computational cell falls dry.	hydrodynamic model	WAQ(2)
delwaq.rtn	File with exit status of WAQ(1) or WAQ(2)	–	–
substate.rtn	(not used)	–	–

A.2 Description of file formats

Some files mentioned in [Table A.1](#) can be/have to be generated by you. Most files are dealt with by the respective programs in D-Water Quality and need not be defined here. You will never have to deal with their formats.

Some files are described elsewhere in the D-Water Quality User Manual:

- 1 <*.lst> Refer to ??.
- 2 <*.lsp> Refer to ??.
- 3 <*.mon> Refer to ??.

A.2.1 Binary files

Binary files are files without any inherent structure. The reading program must take care of properly reading its contents.

A.2.1.1 History files (.his)

This type of file contains the following information:

- ◇ A title consisting of 4 strings of 40 characters *Note:* the fourth string is often used to indicate the date and time of the reference time frame, the so-called T0 string
- ◇ Two integer numbers (4 bytes), the first the number of substances/parameters (NOSYS) and the second the number of locations (NOSEG)
- ◇ The names of the NOSYS substances/parameters, each 20 characters long
- ◇ The names and segment numbers of the selected (monitoring) locations: For each of the NOSEG locations first an integer, being the segment number and then the name, 20 characters again.
- ◇ After this header, each record consists of:
 - the time (in seconds since a reference time)
 - the concentrations/values for all substances/parameter per location

The Fortran code below may be taken as a formal specification:

```
character(len=40), dimension(4)           :: title
character(len=20), dimension(:), allocatable :: parameter_name
character(len=20), dimension(:), allocatable :: location_name
integer, dimension(:), allocatable         :: location_index

real, dimension(:, :), allocatable         :: data
integer                                     :: time
integer                                     :: nosys
integer                                     :: noseq

open( 10, file = history_file, access = 'stream', status = 'old' )
read( 10 ) title
read( 10 ) nosys, noseq

allocate( parameter_name(nosys) )
allocate( location_name(noseq), location_index(noseq) )
allocate( data(nosys,noseq) )

read( 10 ) parameter_name

read( 10 ) ( location_index(i), location_name(i), i = 1,noseq )

do
  read( 10, iostat = ierr ) time, data
```

```

! Or more explicitly:
! read( 10, iostat = ierr ) time, (data(isys,iseg) ,isys = 1,nosys), iseg = 1,noseg)
!

if ( ierr /= 0 ) then
    exit
endif
enddo

```

A.2.1.2 Map files (.map)

This type of file is almost exactly like the history files, except that there are no names for the locations (the number of locations is equal to the total number of segments in the model):

- ◇ A title consisting of 4 strings of 40 characters Note: the fourth string is often used to indicate the date and time of the reference time frame, the so-called T0 string
- ◇ Two integer numbers (4 bytes), the first the number of substances/parameters (NOSYS) and the second the number of locations (NOSEG)
- ◇ The names of the NOSYS substances/parameters, each 20 characters long
- ◇ After this header, each record consists of:
 - the time (in seconds since a reference time)
 - the concentrations/values for all substances/parameter per location

The Fortran code below may be taken as a formal specification:

```

character(len=40), dimension(4)           :: title
character(len=20), dimension(:), allocatable :: parameter_name

real, dimension(:,:), allocatable          :: data
integer                                     :: time
integer                                     :: nosys
integer                                     :: noseg

open( 10, file = map_file, access = 'stream', status = 'old' )
read( 10 ) title
read( 10 ) nosys, noseg

allocate( parameter_name(nosys) )
allocate( data(nosys,noseg) )

read( 10 ) parameter_name

do
    read( 10, iostat = ierr ) time, data

    ! Or more explicitly:
    ! read( 10, iostat = ierr ) time, (data(isys,iseg) ,isys = 1,nosys), iseg = 1,noseg)
    !

    if ( ierr /= 0 ) then
        exit
    endif
enddo

```

A.2.1.3 Segment function files

Segment function files come in two flavours:

- ◇ A binary file with no meta data at all
- ◇ A binary map file as the above, with generally only one parameter

Segment function files have no prescribed file extension. The <*.sal>, <*.tem> and <*.tau> files are examples of segment functions. A segment function is a binary file with space and time varying values for all computational cells. Thus the file is a matrix with dimensions (number of computational cells) and (number of time steps). Segment function can be written with small dedicated programs written in any programming language (e.g. Fortran, C).

The first type can be read as:

```
real, dimension(:,:), allocatable :: data

nosys = ?? ! From outside ...
noseg = ??

open( 10, file = segment_function_file, access = 'stream', status = 'old' )

allocate( data(nosys,noseg) )

do
  read( 10, iostat = ierr ) time, data

  ! Or more explicitly:
  ! read( 10, iostat = ierr ) time, (data(isys,iseq) ,isys = 1,nosys), iseq = 1,noseg)
  !

  if ( ierr /= 0 ) then
    exit
  endif
enddo
```

A.2.1.4 NetCDF files

D-Water Quality can also write map and history files in NetCDF format, for this it needs the name of the corresponding file with the geometric information, the waqgeom-file mentioned in the hyd-file.

The NetCDF output files conform to the so-called UGRID standard (see the UCAR/NetCDF website)

Using such tools as HDFView (for the raw contents) and QuickPlot (for a graphical representation) you can inspect the contents of these files.

See the detailed description of the input file for how this type of output is specified. The user-interface arranges for this automatically.

A.2.1.5 NEFIS files

NEFIS is the name for a legacy library which had much the same purpose as NetCDF. Within the context of the user-interface this type of output is no longer produced.

A.2.2 CSV files for input

CSV files are used by the Delft3D Flexible Mesh Suite or D-HYDRO Suite to import timeseries for boundary conditions and waste loads as well as for process parameters.

The set-up is fairly uniform:

- ◇ The columns are separated by commas (or semicolons, depending on the regional settings).
- ◇ The first line gives the name of the columns, all following lines specify the values.

- ◇ The date/time format is fixed: yyyy/mm/dd HH:MM:SS.
- ◇ All other values on a line are supposed to be ordinary numbers.

For boundary conditions and waste loads the structure is:

- ◇ The name (or better: keyword) for the time is either "timeBlock" or "timeLinear". This identifies the method of interpolating between records.
- ◇ Then follows the location name and the substance name and finally the value.

Here is an example:

```
timeBlock,location,substance,value
2014-01-01 00:00:00,Spill,FLOW,10
2014-02-01 00:00:00,Spill,FLOW,10
2014-01-01 00:00:00,Spill,cTR3,100
2014-02-01 00:00:00,Spill,cTR3,100
2014-01-01 00:00:00,Spill,dTR3,100
2014-02-01 00:00:00,Spill,dTR3,100
```

"FLOW" is a name specific to waste loads and represents the flow rate in m3/s. For boundary conditions no such name is expected (if present it will be ignored).

For boundaries the "location" name is the name of the boundary.

Note: the value -999.0 is reserved as "missing value". If such values are present, the actual value used in the calculation will be determined by interpolation (either as block function or as piecewise linear function).

For process parameters, the file may look like:

```
DateTime,RadSurf
2014/01/01 00:00:00,9.953468
2014/01/07 00:00:00,17.344166
2014/01/14 00:00:00,29.992676
2014/01/21 00:00:00,23.594018
2014/01/28 00:00:00,27.297634
2014/02/04 00:00:00,37.102296
2014/02/11 00:00:00,39.665066
2014/02/18 00:00:00,59.423196
2014/02/25 00:00:00,101.799838
2014/03/03 00:00:00,100.52672
2014/03/10 00:00:00,66.9627
```

So, no location name or parameter name. There may be more than one parameter value per line though, as the user-interface allows you to specify which column to import for the selected parameter.

Important note:

In our experience MicroSoft Excel is a less than perfect tool to create CSV files in the required format, as it often (but not always) outputs the date and time in a different format than the above.

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B The hyd-file

B.1 Contents of the hyd-file

The hyd-file is an ASCII type master file to a hydrodynamic data set that is usually produced by a hydrodynamic program that is connected to D-Water Quality. It contains general information about the hydrodynamic data set such as dimensions, period covered and other slight information. It also contains references to files that contain bulk data. This bulk data is usually in binary form. This chapter contains a description of these files. When provided in the right format, any hydrodynamic program should be able to provide D-Water Quality with such a hydrodynamic data set. In this chapter you can find a description of this file, and the files that come with it.

Example of the content of a hyd-file:

```
file-created-by Deltares, D-Flow FM Version 1.1.212.49841, Feb 11 2017, 18:04:46
file-creation-date 2016-11-14, 11:13:45
task full-coupling
geometry unstructured
horizontal-aggregation no
reference-time '20160805000000'
hydrodynamic-start-time '20160805000000'
hydrodynamic-stop-time '20160806010000'
hydrodynamic-timestep '00000000000100'
conversion-ref-time '20160805000000'
conversion-start-time '20160805000000'
conversion-stop-time '20160806010000'
conversion-timestep '00000000000100'
number-hydrodynamic-layers 10
number-horizontal-exchanges 415
number-vertical-exchanges 888
number-water-quality-segments-per-layer 222
number-water-quality-layers 5
hydrodynamic-file 'f34'
aggregation-file none
boundaries-file 'f34.bnd'
waqgeom-file 'f34_waqgeom.nc'
volumes-file 'f34.vol'
areas-file 'f34.are'
flows-file 'f34.flo'
pointers-file 'f34.poi'
lengths-file 'f34.len'
salinity-file none
temperature-file none
vert-diffusion-file none
horizontal-surfaces-file 'f34.srf'
shear-stresses-file 'f34.tau'
attributes-file 'f34.atr'
hydrodynamic-layers
    0.025000
    0.025000
    0.050000
    0.100000
    0.100000
    0.100000
    0.100000
    0.150000
    0.150000
    0.200000
end-hydrodynamic-layers
water-quality-layers
    3.000000
    1.000000
    2.000000
    2.000000
    2.000000
end-water-quality-layers
```



keyword	value	
file-created-by	string	optional (but strongly recommended) containing e.g. organisation name, program name, version number and/or build date of the program that created this hyd-file
file-creation-date	string	optional (but strongly recommended) preferable format: yyyy-mm-dd hh:mm:ss
task	full-coupling coupling-per-domain	
horizontal aggregation	yes no automatic	
description	'Comment 1' 'Comment 2' 'Comment 3'	optional 3 lines, each line between single quotes
end-description		
geometry	unstructured curvilinear-grid finite-elements z-layers (as an optional second value)	D-Flow FM, UNTRIM Delft3D-FLOW TELEMAC SOBEK-FLOW (not yet defined) D-Flow FM, UNTRIM, Delft3D-FLOW or TELEMAC
reference-time	'yyyymmddhhmmss'	'19920831000000'
hydrodynamic-start-time	'yyyymmddhhmmss'	'19920831000000'
hydrodynamic-stop-time	'yyyymmddhhmmss'	'19920831002000'
hydrodynamic-timestep	'yyyymmddhhmmss'	'00000000000100'
conversion-ref-time	'yyyymmddhhmmss'	'19920831000000'
conversion-start-time	'yyyymmddhhmmss'	'19920831000000'
conversion-stop-time	'yyyymmddhhmmss'	'19920831002000'
conversion-timestep	'yyyymmddhhmmss'	'00000000000100'
grid-cells-first-direction	integer value	structured: number of cells in first direction unstructured: total number of cells
grid-cells-second-direction	integer value	structured: number of cells in second direction unstructured: 1
number-hydrodynamic-layers	integer value	to derive thickness of vertical water quality layers
number-horizontal-exchanges	integer number	required
number-vertical-exchanges	integer number	required
number-water-quality-segments-per-layer	integer number	required
number-water-quality-layers	integer number	required
hydrodynamic-file	'file name' 'name.ddb'	In case of hydrodynamic domain decomposition model
aggregation-file	'name.dwg' none 'per domain'	In case of hydrodynamic domain decomposition model

keyword	value	
grid-indices-file	'name.lga'	curvilinear-grid: required
grid-coordinates-file	'name.cco'	curvilinear-grid: required
boundaries-file	'name.bnd'	unstructured: required
waqgeom-file	'name_waqgeom.nc'	unstructured: required
volumes-file	'name.vol'	required
areas-file	'name.are'	required
flows-file	'name.flo'	required
pointers-file	'name.poi'	required
lengths-file	'name.len'	required
salinity-file	'name.sal'	
	none	
temperature-file	'name.tem'	
	none	
vert-diffusion-file	'name.vdf'	
	none	
horizontal-surfaces-file	'name.srf'	required
dps-file	'name.dps'	optional
discharges-file	'name.src'	optional
chezy-coefficients-file	'name.chz'	
	none	
shear-stresses-file	'name.tau'	optional
walking-discharges-file	'name.wlk'	optional
attributes-file	'name.atr'	required
z-layers-ztop	real	z-layer: required Maximum depth in the model (relative to the reference level; unit: metres; positive upwards).
z-layers-zbot	real	z-layer: required The 'imaginary' maximum water level in the model (relative to the reference level; unit: metres; positive upwards).
minimum-vert-diffusion		
upper-layer	real	
lower-layer	real	
interface-depth	real	
end-minimum-vert-diffusion		
constant-dispersion		
first-direction	real	
second-direction	real	
third-direction	real	
end-constant-dispersion		
hydrodynamic-layers		required
	real	0.4000
	real	0.2500
	real	0.1500
	real	0.1000
	real	0.1000

keyword	value	
end-hydrodynamic-layers		relative thickness of layers, surface to bed level, to derive thickness of vertical water quality layers, one for each hydrodynamic layer
water-quality-layers	real	required
	real	1.0
	real	1.0
	real	1.0
end-water-quality-layer	real	2.0
		number of hydrodynamic layers per water quality layer, to derive thickness of vertical water quality layers, must sum up to the number of hydrodynamic layers
discharges	real or integer	unstructured: <i>x</i> -coordinate structured: first index
	real or integer	unstructured: <i>y</i> -coordinate structured: second index
	integer	layer number
	'discharges name'	name of the discharge
end-discharges	type	values: normal, inlet, outlet, walking
If aggregation-file is 'per domain'		
domains	'name'	domain name
	integer	cell numbers in first direction
	integer	cell number in second direction
end-domains	name.dwg'	aggregation file per domain
If hydrodynamic-file is 'name.ddb'		
dd-boundaries	'name'	domain name 1
	integer	m1
	integer	n1
	integer	m2
	integer	n2
	'name'	domain name 2
	integer	m1
	integer	n1
	integer	m2
end-dd-boundaries	integer	n2

B.2 UGRID files that are directly read by D-Water Quality

<*_flowgeom.nc> (grid)

B.3 ASCII files that are directly read by D-Water Quality

<*.atr-file> (attributes)
<*.bnd-file> (boundary)

B.4 Binary files that are directly read by D-Water Quality

Binary files are very efficient to read. That is why D-Water Quality allows the input from bulky binary files that are written e.g. by the hydrodynamic model that produced flow fields. Many scientific software is written in a flavor of the `FORTRAN` programming language. This makes it very likely that your binary input files for D-Water Quality are written by `FORTRAN`. The `ANSI` standard for that language however does not support binary files. `FORTRAN` supports unformatted files. These are also very efficient to read but they have record information included in the file. This record information is compiler specific so although a standard exists for the unformatted file in the `FORTRAN` language, the contents of that file may vary per implementation. If you are using the same compiler for your hydrodynamic program as was used for our D-Water Quality source code, then there are not so much problems. Before mentioning the name of your binary file in the input file you just give the keyword `UNFORMATTED` and D-Water Quality will open and read the file as an unformatted file. If you are using a very recent compiler, you may open and write your hydrodynamic files with the `ACCESS = 'STREAM'` option in your source code. That is more or less equivalent with the binary files that D-Water Quality is reading normally.

Binary files consist of bit patterns indicating the numbers rather than readable characters. There are several bit patterns around to write integer and real numbers. D-Water Quality is using the IEEE standard with 'little endian' layout of the bytes. That is the common layout on PC type of processors. Main frames and workstations may be equipped with processors that use the 'big endian' layout of bytes. If you are facing those files you may also use the keyword `BIG_ENDIAN` before you specify the name of the binary file to be read by D-Water Quality.

In the following a documentation of the contents of the binary files that are directly read by D-Water Quality is given. This specification also mentions the batches of data that D-Water Quality reads from them separately. This would normally not be of importance. As long as you have written your data in the same order in the binary file, then it does not matter in what chunks D-Water Quality reads them. This is however not the case for unformatted files. They contain record information and the chunks used for reading need to be exactly identical to the chunks used for writing. To support you with that the specification contains the reading procedure.

The table B.2 gives a list of binary files that are read directly by D-Water Quality. Each • indicates a new record for unformatted files. The capital amounts refer to the dimensions mentioned in the corresponding sections of this manual:

Table B.1: Dimensions mentioned in table B.2

Variable	Legenda
NOSEG	Number of computational cells
NOSEGL	Number of active cells in one layer
NOLAY	Number of layers
NOQ1, NOQ2, NOQ3	Number of exchanges in
NOQT	Sum of NOQ1, NOQ2, NOQ3
NODISP	Number of additional dispersion arrays
NOVELO	Number of additional velocity arrays
NOPARAM	Number of parameters that are defined for this file
NSEGFUN	Number of segment functions that are defined for this file Note: the matrix is transposed for this file

Table B.2: Documentation of the binary input files that can be read directly by D-Water Quality

File	Records
exchange pointer (.poi)	<ul style="list-style-type: none"> • 4 integer*4 ifrom, ito, ifrom-1, ito+1 • the same for all other NOQT = NOQ1+NOQ2+NOQ3 exchanges • . . .
exchange lengths (.len)	<ul style="list-style-type: none"> • 'time' integer*4, (2, NOQT) matrix of real*4 values • (1,:) = dx for left/1st cell to interface • (2,:) = dx for interface to right/2nd cell • same for next time step(s) • . . .
horizontal surface (.srf)	<ul style="list-style-type: none"> • 'time (dummy = 0)' integer*4, NOSEG real*4 values • optionally the same for next time step(s) • . . .
segment volumes (.vol), temperature (.tem), tau (.tau), salinity (.sal), vertical diffusion (.vdf)	<ul style="list-style-type: none"> • 'time' integer*4, NOSEG real*4 values • same for next time step(s) • . . .
flows (.flo), exchange areas (.are)	<ul style="list-style-type: none"> • 'time' integer*4, NOQT real*4 values • same for next time step(s) • . . .
segment functions (*.*)	<ul style="list-style-type: none"> • 'time' integer*4, (NOSEG, NSEGFUN) matrix of real*4 values • same for next time step(s) • . . .

C Standard substance files

C.1 Introduction

For the analysis of water quality problems it is often useful to proceed in steps. The starting point might be substances like salinity (for coastal and estuarine areas) and tracers, as they give an impression of the transport and residence time in a water system. Just knowing how fast substances are transported from a source to a target area means you can concentrate on those processes that have a comparable time scale. For instance: if the time for water to travel from the source to the target area is one month, then it is very unlikely that bacterial pollution at that source will be of interest at that target area: bacteria die in a matter of hours, when released into the environment.

The next step could be to study the effect of organic material on oxygen – if there is an indication that there are problems with oxygen. Using a simple set-up for such a problem, with BOD and DO as the only substances, gives you a first impression as to where oxygen problems may occur and under what circumstances. There would be no need to collect data on nutrients and algae, as well as organic waste, before you can do a useful calculation.

Of course nutrients may be of importance as well. In that case you have a choice: use a model set-up that includes algal growth or simply force a particular concentration of algae and see what effect they have on nutrients.

To help you setting up a water quality model, from very simple to more sophisticated, several substance files, containing a selection of substances, processes working on these substances and relevant process parameters are available. The following sections contain a description of the standardised substance files:

- ◇ Salinity and tracers (fractions)
- ◇ A basic coliform model
- ◇ A basic dissolved oxygen model, and
- ◇ A basic suspended matter model.

These substance files <*.sub> can be used as they are but they can also serve as basis for a more extensive water quality simulation. Use the corresponding PLCT files <*.0> to expand them with more substances and processes.

Note: The files themselves can be found in the directory with tutorial data.

C.2 Salinity and tracers (fractions)

C.2.1 General

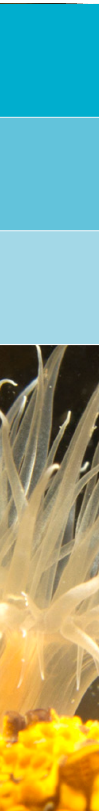
The Salinity and Tracers Model is a *predefined* set of selected state variables, active processes, editable input and output parameters. It has been constructed with the Processes Library Configuration Tool and experienced users may use the same tool to edit the predefined set. This describing document is linked to the files:

Name of PLCT input file	<salinity_tracers.0>
Name of substance file	<salinity_tracers.sub>

C.2.2 Introduction

This set of substances and processes is meant for a first impression of the dynamics of the system:

- ◇ Salinity is a conservative substance and indicates the mixing of seawater with fresh water inputs. Useful for marine and estuarine environments. For fresh water systems this is not usually relevant.
Note: Salinity is often included in the hydrodynamic model as well. Ideally the results from the hydrodynamic model and those from the water quality model should be identical, but differences in the underlying numerical methods may cause differences.
- ◇ Conservative tracers 1 and 2 can be associated with specific sources to study how fast water from these sources is spread by the flow. They can also be used to see how much water of the source reaches a particular area.
Besides point sources like rivers flowing into a lake or discharges via a pipe into the sea you can also regard the open boundary of the model area as a source: just set the concentration to a value like 1 or 100.



- ◇ When combining with the decayable tracers use the same input (boundary values, waste loads) for both the conservative and the decayable tracer. The output from the Age process will then show how long it takes for the water from the source to reach a particular area in the model or the residence time for the model region as a whole.

Note: The decay coefficient must be chosen so that the reciprocal is of the same order as the residence time. For instance: a lake with a residence time (the time in which the water will be refreshed by incoming rivers and the like) of 2 months requires a decay coefficient in the order of $1/(2 \cdot 30) = 0.017/\text{day}$. That is: 0.005/day would do as well as 0.05/day, but not 1/day.

C.2.3 Description of processes

The only processes that are selected in this case are the decay of the decayable tracers and the determination of the "age" for water containing the conservative and decayable tracer from a particular source.

The first process is implemented as first-order decay:

$$\frac{d[Trace_i]}{dt} = -k_{decay}[Trace_i] \quad (C.1)$$

To determine the "age" T of the water as it has come from the source:

$$T_i = -\frac{1}{k_{decay}} \ln([dTrace_i]/[cTrace_i]) \quad (C.2)$$

Input item	Description	Unit	Default value	Editable	Range
$[cTrace_i]$	concentration of conservative tracer i	$g.m^{-3}$	n.a. (state variable)	n.a.	—
$[dTrace_i]$	concentration of decayable tracer i	$g.m^{-3}$	n.a. (state variable)	n.a.	—
$k_{decay,i}$	decay rate coefficient for decayable tracer i	d^{-1}	yes	0.001-0.1	—
T_i	"age" (travel time) of tracer i	d	output of process	—	—

C.2.4 Notes

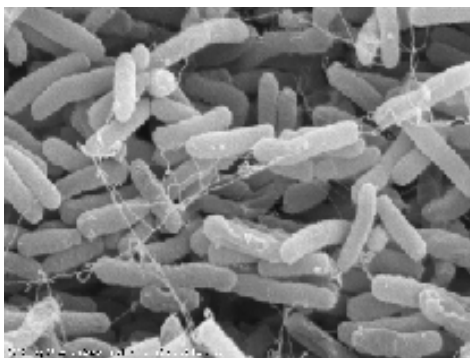
- ◇ To determine the "age" the conservative tracer and the corresponding decayable tracer must have the same initial and boundary concentration and have the same concentration in the discharges. The actual value is typically chosen 1 or 100, but it does not really matter.
- ◇ If you are not interested in the "age", then the four tracers can be used independently.

C.2.5 Output items

Apart from the concentration of the state variables, the following parameters are available as extra output:

Parameter id	Description	Unit	Model name
T_1	Age as calculated from the first pair of tracers	d^{-1}	Age1
T_2	Age as calculated from the second pair of tracers	d^{-1}	Age2

C.3 Basic coliform model



C.3.1 General

The Basic Coliform Model is a *predefined* set of selected state variables, active processes, editable input and output parameters. It has been constructed with the Processes Library Configuration Tool and experienced users may use the same tool to edit the predefined set. This describing document is linked to the files:

Name of PLCT input file	<coli_04.0>
Name of substance file	<coli_04.sub>

C.3.2 Introduction

Coliform bacteria originate from human and animal faeces and are often used as indicator for the presence of disease factors. The coliform group of bacteria comprises all aerobic and facultative anaerobic, gram-negative, nonspore-forming, rod-shaped bacteria that ferment lactose with gas formation within 48 hr at 35 °C (Thomann and Mueller, 1987). *Escherichia coli* is the best known member of this group.

As soon as coliform bacteria have been discharged into surface water, they start to die since the conditions that these bacteria meet, are essentially hostile to them. The mortality of coliform bacteria is enhanced by temperature, salinity and solar radiation. The lethal effect of light is associated with short wavelengths, ultraviolet radiation in particular.

The table below gives an overview of the selected state variables and processes.

Substance Group	State variable	Model name	Processes
Coli-Bacteria	<i>Escherichia coli</i>	EColi	Mortality EColi bacteria
General	Salinity	Salinity	–
Suspended Matter	Inorganic matter (cohesive sediment)	IM1	–
Extra processes			
<ul style="list-style-type: none"> ◇ Extinction of ultraviolet light ◇ UV-Radiation at segment upper and lower boundary ◇ Calculation of chloride concentration 			

C.3.3 Description of processes

For a formal description refer to the Technical Reference Manual (TRM) for the individual processes of the Processes Library.

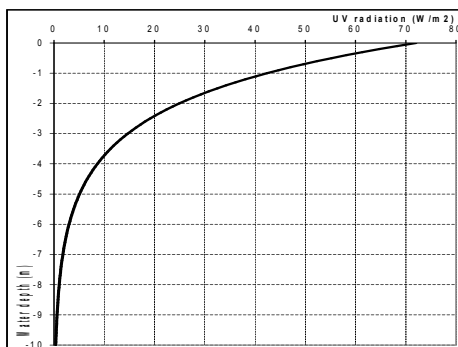
The mortality rate of *E. Coli* depends on the ambient salinity (or chloride concentration), temperature and the intensity of the UV radiation.

$$Flux = \left((Rc_0 + Mrt_{Cl}) \times \vartheta^{T-20} + Mrt_{Rad} \right) \times [E.Coli] = Mrt_{E.Coli} \times [E.Coli]$$

$$Mrt_{Cl} = k_{Cl} \times [Cl]$$

$$Mrt_{Rad} = Rc_{Rad} \times DL \times I \times f_{UV} \times \frac{1 - e^{(-Ext_{UV} \times H)}}{Ext_{UV} \times H}$$

Input item	Description	Unit	Default value	Editable	Range
[<i>E.Coli</i>]	concentration of coliform bacteria	MPN.m ⁻³	n.a. (state variable)	n.a.	–
<i>DL</i>	day length	d	0.58	yes	depends on latitude and season
<i>Ext_{UV}</i>	total extinction of UV-radiation	m ⁻¹	derived from process	n.a.	–
<i>f_{UV}</i>	fraction of UV-radiation in visible light	-	0.12	no	–
<i>H</i>	water depth	m	derived from process	n.a.	–
<i>I</i>	solar radiation at segment upper boundary	W.m ⁻²	derived from process	n.a.	–
<i>k_{Cl}</i>	chloride related mortality constant	m ³ .g ⁻¹ .d ⁻¹	1.1·10 ⁻⁵	no	–
<i>Mrt_{Cl}</i>	chloride dependent mortality rate	d ⁻¹	n.a.	n.a.	–
<i>Mrt_{Rad}</i>	radiation dependent mortality rate	d ⁻¹	n.a.	n.a.	–
<i>Mrt_{E.Coli}</i>	total mortality rate of <i>E.Coli</i>	d ⁻¹	n.a.	n.a.	–
<i>Rc₀</i>	first order mortality rate	d ⁻¹	0.8	yes	0.8 - 5.0
<i>Rc_{Rad}</i>	radiation related mortality constant	m ² .W ⁻¹ .d ⁻¹	0.086	no	–
<i>ϑ</i>	temperature coefficient of the mortality rate	-	1.07	no	–
<i>T</i>	temperature	°C	15	yes	depends on local conditions
[<i>Cl</i>]	chloride concentration	g.m ⁻³	derived from process	n.a.	–



The chloride concentration is derived from the salinity. The water depth is defined by the model schematisation. The solar radiation at the upper segment boundary is calculated from the total surface radiation at the water surface and the extinction in the segments above (see figure to the right). The extinction of UV-light depends on the suspended matter concentration and a background extinction according to:

$$Ext_{UV} = Ext_{Bak} + Ext_{IM1} \times [IM1]$$

$$I = I_0 \times e^{-Ext_{UV} \times H}$$

Input item	Description	Unit	Default value	Editable	Range
Ext_{UV}	total extinction of UV-radiation	m^{-1}	n.a.	n.a.	—
Ext_{Bak}	background extinction	m^{-1}	0.08	yes	0.08 - 1.0
Ext_{IM1}	extinction coefficient of inorganic suspended matter	$m^2.g$	0.01	yes	0.01 - 0.05
$[IM1]$	concentration of inorganic suspended matter	$g.m^{-3}$	n.a. (state variable)	n.a.	—
I_0	total radiation at the water surface	$W.m^{-2}$	160	yes	depends on latitude and season
I	solar radiation at segment upper boundary	$W.m^{-2}$	n.a.	n.a.	—
H	water depth	m	n.a.	n.a.	—

C.3.4 Notes

- ◇ Pure water has an extinction of $0.08 m^{-1}$ and this is considered the background extinction. The Basic Coliform Model has only one other constituent that contributes to the extinction, namely inorganic suspended matter. Other constituents — mainly the organic components — are ignored. A higher background extinction can be used to compensate this.
- ◇ Approximately 6 percent of the total solar radiation reaching the earth's surface is in the UV range. That is approximately 12 percent of solar radiation measured as visible light, because visible light is approximately 50 percent of total light. The water quality model requires input of the total solar radiation at the water surface as the total visible light intensity, which will be scaled (using the f_{UV} constant) to the UV radiation internally. Radiation is often available in the units MJ/m^2 , where the irradiation is accumulated over a day; the conversion factor between $MJ m^{-2}$ per day and $W m^{-2}$ is 11.57 ($= 10^6/86400$).
- ◇ Settling of the cohesive sediment ($IM1$) is ignored in the Basic Coliform Model.

C.3.5 Output items

Apart from the concentration of the state variables, the following parameters are available as extra output:

Parameter id	Description	Unit	Model name
Ext_{UV}	total extinction of UV-radiation	m^{-1}	ExtUV
$MrtE.Coli$	total mortality rate of <i>E.Coli</i>	d^{-1}	MrtToEColi

C.4 Basic dissolved oxygen model

The Basic Dissolved Oxygen Model is a *predefined* set of selected state variables, active processes, editable input and output parameters. It has been constructed with the Processes Library Configuration Tool and experienced users may use the same tool to edit the predefined set. This describing document is linked to the files:

Name of PLCT input file	<oxy_general_04.0>
Name of substance file	<oxy_general_04.sub>

C.4.1 Introduction

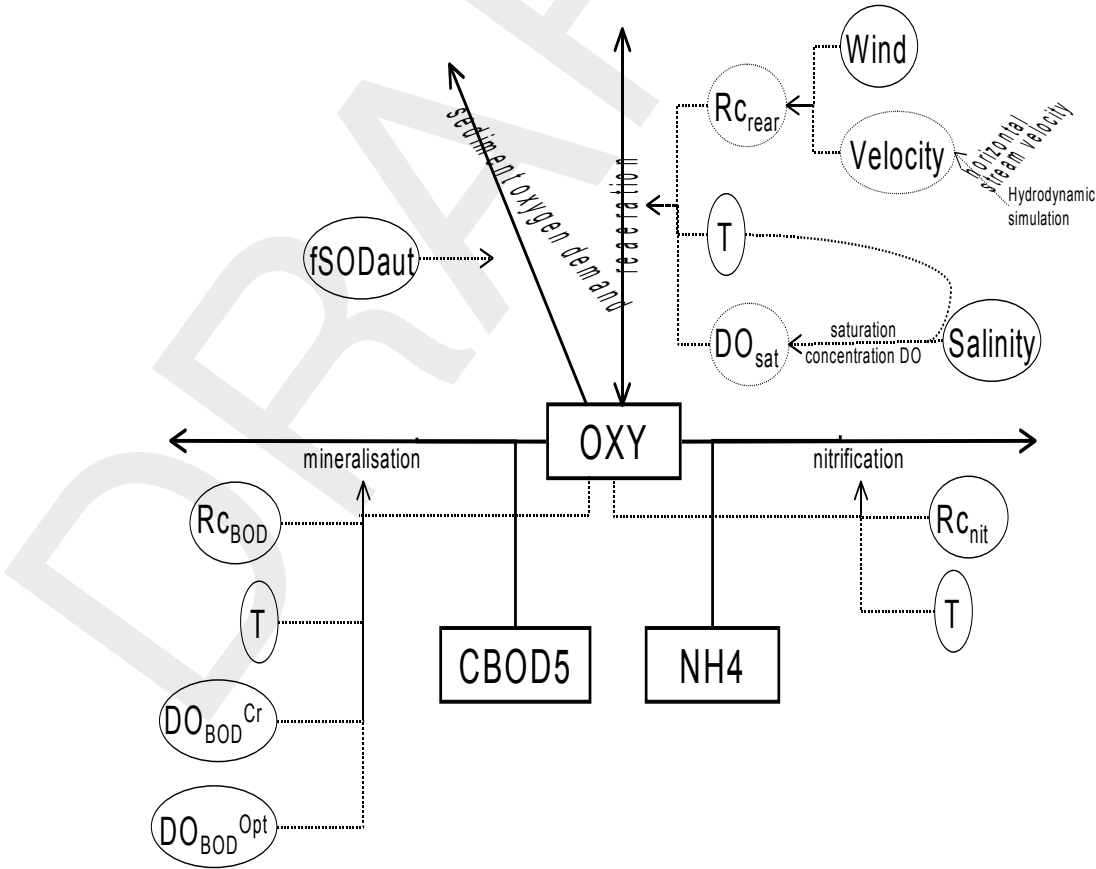
Low dissolved oxygen (DO) concentrations are often associated with bad water quality. However, low dissolved oxygen concentrations can occur due to natural conditions as well, when stratification isolates the hypolimnion (the part of the water column below the pycnocline) from the atmosphere. For example, as a result of a permanent stratification the Black Sea has no dissolved oxygen from a depth of approximately 200 metres down. Consumption of dissolved oxygen – in general mainly for the decay of organic matter – lowers the concentration, without the possibility of replenishment from the atmosphere.

The anthropogenic impact on dissolved oxygen can be two-way. The discharge of the effluent of sewage treatment works or even the discharge of untreated sewerage, brings organic matter in the environment. If the assimilation capacity of the natural system is exceeded, the dissolved oxygen concentration may fall to detrimental levels. A second pathway of low dissolved concentrations is more indirect. In eutrophic systems where nutrient levels have been increased considerably, algal blooms can produce large amount of organic matter which in turn through their decay lower the dissolved oxygen concentration.

The Basic Dissolved Oxygen Model is loosely based on the classic Streeter-Phelps formulation which was derived for a continuous BOD load to a river ([Streeter and Phelps, 1925](#)). Apart from dissolved oxygen itself, two state variables are included: organic matter as BOD and ammonium. The Basic Dissolved Oxygen Model simulates the decay of organic matter, nitrification of ammonium and replenishment of dissolved oxygen through reaeration. The table below gives an overview of the selected state variables and processes. The flow chart on this page shows the connection between state variables, processes and process parameters.

Substance Group	State variable	Model name	Processes
COxygen-BOD	Dissolved oxygen BOD5 (carbonaceous)	OXY CBOD5	Mineralisation of BOD Reaeration
Eutrophication	Ammonium	NH4	Nitrification
Extra processes			
<ul style="list-style-type: none"> ◇ Sediment oxygen demand ◇ Saturation concentration dissolved oxygen ◇ Horizontal stream velocity ◇ Calculation of chloride concentration 			

General Dissolved Oxygen Model



C.4.2 Description of processes

For a formal description refer to the Technical Reference Manual (TRM) for the individual processes of the Processes Library.

Mineralisation of BOD

Carbonaceous BOD is subject to a linear and temperature and oxygen dependent decay process:

$$\text{Mineralisation flux} = -R_{CBOD} \times [CBOD5] \times \vartheta_{BOD}^{(T-20)} \times \frac{[O_2] - DO_{BOD}^{Cr}}{DO_{BOD}^{Opt} - DO_{BOD}^{Cr}} \quad (C.3)$$

Input item	Description	Unit	Default value	Editable	Range
[CBOD5]	Concentration of carbonaceous BOD5	gO ₂ .m ⁻³	n.a. (state variable)	n.a.	–
R_{CBOD}	First order rate constant at 20 °C	d ⁻¹	0.3	yes	0.1 - 2.0
ϑ_{BOD}	Temperature coefficient	-	1.04	no	–
T	Water temperature	°C	15	yes	depends on local conditions
[O ₂]	Dissolved oxygen concentration	gO ₂ .m ⁻³	n.a. (state variable)	n.a.	–
DO_{BOD}^{Cr}	Critical dissolved oxygen concentration for BOD mineralisation	gO ₂ .m ⁻³	1	yes	0 - 1
DO_{BOD}^{Opt}	Optimal dissolved oxygen concentration for BOD mineralisation	gO ₂ .m ⁻³	5	yes	0 - 5

Nitrification

Nitrification is the conversion of ammonium to nitrate. The stoichiometry of the reaction is ($NH_4^+ : O_2 : NO_3^- = -1 : -4.571 : 1$) with concentrations in gN.m⁻³, gO₂.m⁻³ and gN.m⁻³ respectively.



The nitrification process is formulated linearly and temperature and oxygen dependent:

$$\text{Nitrification flux} = -R_{nit} \times [NH_4] \times \vartheta_{nit}^{(T-20)} \times \frac{[O_2] - DO_{nit}^{Cr}}{DO_{nit}^{Opt} - DO_{nit}^{Cr}} \quad (C.5)$$

Input item	Description	Unit	Default value	Editable	Range
[NH ₄]	Concentration of ammonium	gN.m ⁻³	n.a. (state variable)	n.a.	–
R_{nit}	First order rate constant for nitrification at 20 °C	d ⁻¹	0.1	yes	–
ϑ_{BOD}	Temperature coefficient	-	1.07	no	–
T	Water temperature	°C	15	yes	depends on local conditions
[O ₂]	Dissolved oxygen concentration	gO ₂ .m ⁻³	n.a. (state variable)	n.a.	–
DO_{nit}^{Cr}	Critical dissolved oxygen concentration for BOD mineralisation	gO ₂ .m ⁻³	1	no	0 - 1

Input item	Description	Unit	Default value	Editable	Range
DO_{nit}^{Opt}	Optimal dissolved oxygen concentration for BOD mineralisation	$\text{gO}_2 \cdot \text{m}^{-3}$	5	no	0 - 5

Nitrification stops when the water temperature drops below a certain critical level, which is by default assumed to be 3 °C. Also, it is supposed to proceed under aerobic conditions only. Therefore, the process flux depends on the dissolved oxygen concentration. If the oxygen concentration is about 5 mg/l (DO_{nit}^{Opt}), the process proceeds without limitation. If the oxygen concentration is below 1 mg/l (DO_{nit}^{Cr}), the process stops completely. If the oxygen concentration is between 1 and 5 mg/l, the limitation factor varies linearly between 0 and 1.

Reaeration

Reaeration is formulated as a first order process working on the oxygen deficit:

$$\text{Reaeration flux} = R_{c_{rear}} \times (DO_{sat} - [O_2]) \times \vartheta_{rear}^{(T-20)} \quad (\text{C.6})$$

$$R_{c_{rear}} = f(\text{wind speed, stream velocity, water depth}) = f(Sw_{rear}) \quad (\text{C.7})$$

$$DO_{sat} = f(T, \text{salinity}) \quad (\text{C.8})$$

Input item	Description	Unit	Default value	Editable	Range
$R_{c_{rear}}$	First order reaeration rate constant	d^{-1}	n.a. (internal variable)	n.a.	–
DO_{sat}	Saturation concentration of dissolved oxygen	$\text{gO}_2 \cdot \text{m}^{-3}$	derived from process	n.a.	–
$[O_2]$	Dissolved oxygen concentration	$\text{gO}_2 \cdot \text{m}^{-3}$	n.a. (state variable)	n.a.	–
ϑ_{rear}	Temperature coefficient for reaeration	-	1.016	no	–
T	water temperature	°C	15	yes	depends on local conditions
Sw_{rear}	Switch for reaeration formulation	-	1	yes	1-7, 9-11

Wind speed and salinity are input parameters and, obviously, depend on local conditions. The stream velocity can be derived from the hydrodynamic model using the process 'Horizontal stream velocity'. Water depth will be derived from the hydrodynamic model as well.

Reaeration depends on the wind speed, the stream velocity and the water depth. In rivers the stream velocity usually provides the major contribution to the reaeration rate constant. In lakes, estuaries and coastal areas stream velocities are generally lower than in rivers and wind speed takes over as the main contributor. For this reason there are in total 10 formulations for the reaeration rate constant in D-Water Quality, indicated by the Sw_{rear} switch. In rivers, you can use the default formulation. Otherwise, Sw_{rear} has to be set to 7 or 9 to include the influence of wind. Both formulations are equally applicable.

Sediment Oxygen Demand

The 'Sediment oxygen demand' process allows you to specify an additional oxygen consumption by the sediment. The input variable is called $fSOD_{aut}$ and has the unit of $\text{g} \cdot \text{m}^{-2} \cdot \text{d}^{-1}$. This process can proceed under aerobic conditions in the water column only. If the oxygen concentration is over 2 mg/l, the process proceeds without limitation. If the oxygen concentration is equal to or below 0 mg/l, the process stops completely. If the oxygen concentration is between 0 and 2 mg/l, the limitation factor varies linearly between 0 and 1.

C.4.3 Notes

It is possible to reach a negative dissolved oxygen concentration in the model, if the consumption of oxygen is allowed to proceed below 0 mg/l. This is only possible if one or more of the critical dissolved oxygen concentrations is given a negative value. A negative dissolved oxygen concentration can be considered as representing reduced substances such as methane or sulphides

C.4.4 Output items

Apart from the state variables, the following parameters are available as extra output:

Parameter id	Description	Unit	Model name
R_{crear}	Reaeration rate constant	d^{-1}	RCREAR
DO saturation percentage	Saturation percentage of dissolved oxygen	%	SatPercOXY
DO saturation concentration	Saturation concentration of dissolved oxygen	$gO_2.m^{-3}$	SaturOXY
Stream velocity	Horizontal stream velocity	$m.s^{-1}$	Velocity

C.5 Basic suspended sediment model

C.5.1 General

The Basic Suspended Sediment Model is a *predefined* set of selected state variables, active processes, editable input and output parameters. It has been constructed with the Processes Library Configuration Tool and experienced users may use the same tool to edit the predefined set. This describing document is linked to the files:

Name of PLCT input file	<sed_1fraction_04.0>
Name of substance file	<sed_1fraction_04.sub>

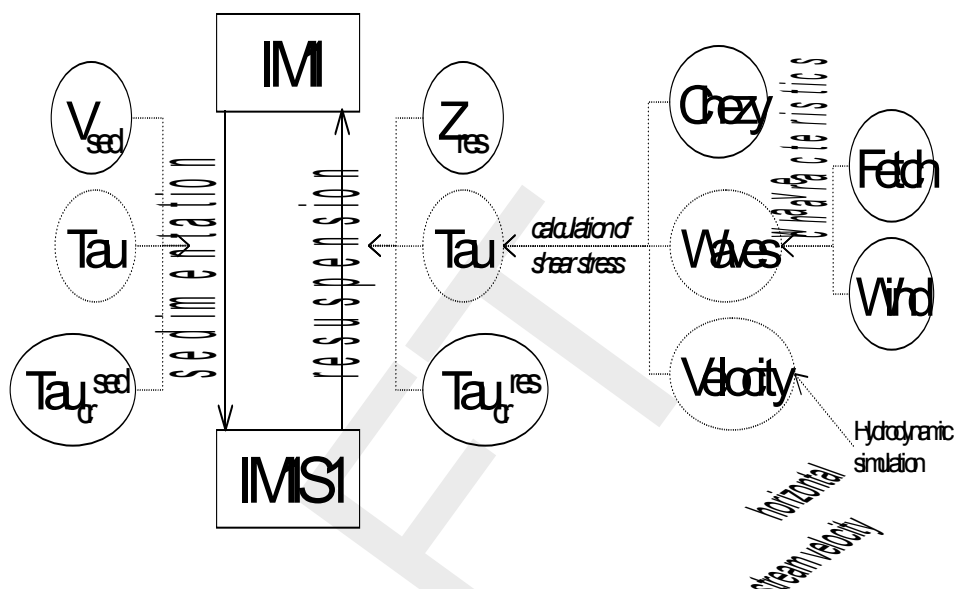
C.5.2 Introduction

Suspended sediment is one of the easiest recognisable water quality parameters and one of the most important for that matter. Suspended sediment, also often referred to as suspended (particulate) matter, is generally associated with two major water quality issues:

- 1 Underwater light climate. Availability of light is essential for primary production. In highly turbid water primary production is suppressed, while in clear waters lush underwater vegetation can develop (if other conditions such as nutrients are met).
- 2 Sedimentation and erosion. Millions of tons of sediment are dredged each year around the world to keep sea-ways and harbours navigable for ships. Obviously, the rate of sedimentation in these economically important regions is of interest to authorities. On the other hand, either at the dredging location or at a dumping site suspended sediment is released during dredging, which may impact the nearby ecosystem.

The Basic Suspended Sediment Model contains a single suspended sediment fraction called IM1 which stands for Inorganic Matter 1st fraction. D-Water Quality allows you to include up to three inorganic matter fractions. The Basic Suspended Sediment Model enables you to simulate the dispersion of suspended sediment taking into account sedimentation and erosion. Additionally, the Secchi disk depth is calculated to assess the effect on the underwater light climate.

The table below gives an overview of the selected state variables and processes. The flow chart on the top of this page shows the connection between state variables, processes and process parameters.



Substance Group	State variable	Model name	Processes
Suspended Matter	Inorganic Matter (suspended)	IM1	Sedimentation
	Inorganic Matter in the sediment (settled)	IM1S1	Erosion
Extra processes			
<ul style="list-style-type: none"> ◇ Total resuspension ◇ Composition of sediment layer S1 ◇ Calculation of bottom shear stress (Tau) ◇ Wave characteristics ◇ Horizontal stream velocity ◇ Calculation of Secchi Depth ◇ Extinction of visible light 			

C.5.3 Description of processes

For a formal description refer to the Technical Reference Manual (Deltares, 2024e) for the individual processes of the Processes Library.

C.5.4 Inorganic Matter (suspended and settled)

The concentration of suspended sediment in the water column (state variable $IM1$) decreases when sedimentation occurs. Erosion, alternatively called resuspension, increases the suspended sediment concentration in the water column. Obviously, the opposite holds for the amount settled on the bottom (state variable $IM1S1$). Together, $IM1$ and $IM1S1$ form a closed mass balance. The well-known Partheniades-Krone formulations for sedimentation/erosion are implemented in D-Water Quality.

The sedimentation of $IM1$ depends on the bottom shear stress (Tau) and a user-defined critical shear stress for sedimentation (Tau_{cr}^{sed}). Only if the bottom shear stress is lower than the critical shear stress for sedimentation, sedimentation occurs:

$$Sedimentation\ flux = P_{sed} \times V_{sed} \times [IM1] \quad (C.9)$$

$$P_{sed} = \max \left(0, 1 - \frac{Tau}{Tau_{cr}^{sed}} \right) \quad (C.10)$$

Input item	Description	Unit	Default value	Editable	Range
[IM1]	concentration of Inorganic Matter 1	g m^{-3}	n.a. (state variable)	n.a.	–
P_{sed}	Probability for sedimentation	-	n.a. (internal variable)	n.a.	0 - 1
V_{sed}	Settling velocity	m d^{-1}	0.1	yes	0.1 - 10
Tau	Bottom shear stress	N m^{-2}	derived from process	n.a.	–
Tau_{cr}^{sed}	Critical shear stress for sedimentation	N m^{-2}	0.1	yes	0.01 - 2.0

Resuspension depends on the bottom shear stress and a user-defined critical shear stress for resuspension (Tau_{cr}^{res}). Only if the bottom shear stress is higher than the critical shear stress for resuspension, resuspension occurs:

$$Resuspension\ flux = P_{res} \times Z_{res} \quad (C.11)$$

$$P_{res} = \max \left(0, \frac{Tau_{cr}^{res}}{Tau} - 1 \right) \quad (C.12)$$

Input item	Description	Unit	Default value	Editable	Range
P_{res}	Probability for resuspension	-	n.a. (internal variable)	n.a.	0 – 1
Z_{res}	Zero-order resuspension rate	$\text{g m}^{-2} \text{d}^{-1}$	0	yes	100 – 100,000
Tau	Bottom shear stress	N m^{-2}	derived from process	n.a.	-
Tau_{cr}^{res}	Critical shear stress for resuspension	N m^{-2}	0.1	yes	0.05 – 2.0

The resuspension flux acts on the total amount of dry matter in the sediment. In the Basic Suspended Sediment Model the state variable *IM1S1* constitutes the total amount as we have no other particulate components. However, in more extensive applications two more inorganic matter components and several organic matter components can be included. Then the resuspension flux of the individual components is proportional to the available fraction in the sediment (e.g. if the mass fraction of *IM1S1* is 10 % and the total resuspension flux is $100 \text{ g m}^{-2} \text{d}^{-1}$, then the resuspension flux of *IM1S1* is $10 \text{ g.m}^{-2}.\text{d}^{-1}$). These fractions are calculated by the process 'Composition of sediment layer S1'.

The bottom shear stress, Tau , represents the force exerted on the sediment by flowing water and wave action.

$$Tau = Tau_{veloc} + Tau_{waves} \quad (C.13)$$

$$Tau_{veloc} = f(\text{stream velocity, Chezy}) \quad (C.14)$$

$$Tau_{waves} = f(\text{wind speed, water depth, Fetch}) \quad (C.15)$$

Input item	Description	Unit	Default value	Editable	Range
Tau_{veloc}	Shear stress exerted by stream velocity	N.m^{-2}	n.a. (internal variable)	n.a.	–
Tau_{waves}	Shear stress exerted by waves	N.m^{-2}	n.a. (internal variable)	n.a.	–
<i>Chezy</i>	Chézy coefficient	$\text{m}^{1/2} \text{s}^{-1}$	no default	yes	40 – 60
<i>Fetch</i>	Fetch length for the wind	m	no default	yes	depends on area

The stream velocity can be derived from the hydrodynamic model using the process 'Horizontal stream velocity'. Wind speed, water depth and Fetch are used in the process 'Wave characteristics' to calculate the typical wave height, wave period and wave amplitude, which in turn determine the shear stress exerted by waves. The wind speed is in input parameter and is often derived from measurements. Usually, a time series with a frequency of once per hour or once per day is applied.

The Basic Suspended Sediment Model also calculates the Secchi Depth (in metres).

$$Secchi\ Depth = \frac{PA_{constant}}{Ext_{VI}} \quad (C.16)$$

$$Ext_{VI} = Ext_{VI}^{Bak} + Ext_{VI}^{IM1} \times (IM1) \quad (C.17)$$

Input item	Description	Unit	Default value	Editable	Range
Ext_{VI}	Total extinction of Visible Light	m^{-1}	n.a.	n.a.	—
$PA_{constant}$	Poole-Atkins constant	-	1.7	no	—
Ext_{VI}^{Bak}	Background extinction for Visible light	-	0.08	yes	0.08 – 1.0
Ext_{VI}^{IM1}	Specific VI extinction of $IM1$	$m^2\ g^{-1}$	0.01	yes	0.01 – 0.05
$[IM1]$	Concentration of Inorganic Matter 1	$g\ m^{-3}$	n.a. (state variable)	n.a.	—

C.5.5 Notes

- ◇ The settling velocity can be made dependent on salinity, total suspended sediment concentration (to account for flocculation) and temperature.
- ◇ Pure water has an extinction of $0.08\ m^{-1}$ and this is considered the background extinction. The Basic Suspended Sediment Model has only one other constituent that contributes to the extinction, namely Inorganic (suspended) Matter. Other constituents — mainly the organic components — are ignored. A higher background extinction should be used to compensate this.

C.5.6 Output items

Apart from the concentration of the state variables, the following parameters are available as extra output:

Parameter id	Description	Unit	Model name
Tau	Bottom shear stress	$N\ m^{-2}$	Tau
<i>Sedimentation flux</i>	Sedimentation flux of $IM1$	$g\ m^{-2}\ d^{-1}$	fSedIM1
<i>Resuspension flux</i>	Total resuspension flux	$g\ m^{-2}\ d^{-1}$	fResS1DM
Ext_{VI}	Total extinction of Visible light	m^{-1}	ExtVL
<i>Secchi Depth</i>	Secchi disk depth	m	SecchiDept
<i>Stream velocity</i>	Horizontal stream velocity	$m\ s^{-1}$	Velocity

C.6 References

The references used in this appendix are:

- section C.3: Thomann and Mueller (1987)
- section C.4: Streeter and Phelps (1925)
- section C.5: Krone (1962); Partheniades (1962); Poole and Atkins (1929)

DRAFT

D Statistical output functions

D-Water Quality offers a number of statistical output facilities as described in Chapter ???. This section describes the individual functions in more detail and provides some hints as to their use. For each function the kind of output is described as well as the options that control the output.

Function	Output parameters	Output files
Stadsc	Average (prefix: MEAN_) Maximum (MAX_) Minimum (MIN_) Standard deviation (STDEV_)	Statistical map and monitor files
Stageo	Geometrical mean (GEO_)	Statistical map and monitor files
Stadpt	Depth-averaged values (DPTAVG_) Minimum over depth (DPTMIN_) Maximum over depth (DPTMAX_)	Ordinary output files
Staday	Periodic mean (TAVG_)	Ordinary output files
Staqt1	Quantile (QUANT_)	Statistical map and monitor files
Staprc	Percentage of exceedance (PERC_) Mean concentration during exceedance (CMN_)	Statistical map and monitor files

D.1 Descriptive statistical parameters (stadsc)

The basic statistical parameters include:

- ◇ The average value and the standard deviation over a chosen period.
- ◇ The maximum and minimum value over that period.

For each water quality parameter these four quantities are computed over all the defined periods. As by definition there is only one result (per period) for the whole simulation, the quantities are written to a separate map and to a separate monitor file (both with the suffix "-stat"). There is no corresponding history output (with only one time this makes very little sense).

Options:

None

D.2 Geometric mean (stageo)

For quantities whose distribution is very skewed, like the concentration of bacteria or suspended solids, a more useful measure to characterise the values may be the *geometrical mean*:

$$C_{geo} = (C_1 \cdot C_2 \cdot C_3 \cdot \dots \cdot C_n)^{1/n}$$

The geometrical mean is only defined for *positive* values (it can be interpreted as the side of a hypercube with the same volume as the hyperblock with sides C_1, C_2, \dots). To make sure very low values do not dominate the outcome, the function as implemented uses a *threshold*: any value below the threshold is set equal to that threshold before it enters the computation.

As with the descriptive statistics function the averaging takes place over the defined period and the output is written to the statistical map and monitor files.

Options:

threshold:

Values below the threshold are reset to the threshold value to avoid run-time errors and too large an influence on the result of very low values.

Bucket	Number of values	Cumulative number
<1	10	10
1–2	20	30
2–3	20	50
3–4	20	70
>4	10	80

D.3 Depth-average mean (stadpt)

Averaging can take place over time, but also over spatial dimensions. The most common type of spatial averaging is the averaging over depth. The output parameter is written to the ordinary files. The only difference with the regular output is that the values are repeated over the layers. Along with the average, the output function also determines the minimum and the maximum of the parameter over depth.

Options:

None

D.4 Periodical mean (staday)

With the descriptive statistics you get an overview of the water quality parameters for given periods. It is also possible however to determine the daily mean for such parameters or the mean for any period that is of interest. This is done with the *staday* function. The output behaves as an ordinary time-dependent variable, with the exception that it is only updated at the end of each period. The output is written to the ordinary output files.

Options:

period: The period over which to average (in seconds).

D.5 Quantiles (staqtl)

Some water quality standards are defined in terms of *quantiles*: for instance the concentration of bacteria may exceed some value only 10 % of the time. This can be determined directly (via the function *staprc*) or the 90 % quantile (percentage) can be determined: the value that is exceeded only 10 % of the time.

The computation of this quantity is fairly complicated:

- ◇ First the probable bounds for the concentrations of the water quality parameter in question are determined *a priori*, that is, they must be set prior to the beginning of the water quality computation. These bounds together with the number of buckets are used to set up "buckets" or classes for the concentration.
- ◇ Then during the computation (taking the period of interest into account) the actual concentrations are classified and the number of values in the corresponding bucket is increased.
- ◇ At the end of the period of interest the histogram that has been calculated in this way is examined to determine an estimate of the quantile. Suppose for instance that the 75 % quantile is sought and five buckets are used, with minimum and maximum respectively 1 and 4:
- ◇ There are 80 observations, so the 75 % quantile occurs within the fourth bucket (we must determine the threshold below which 60 of the computed values occur). Linear interpolation is used to estimate that threshold: the quantile is approximately 3.5.

The accuracy of these estimates depends greatly on the chosen range, the number of buckets and the quantile that is looked for:

- ◇ If the range is chosen wrongly, most values will fall into a few buckets. As there is no information on the distribution within a bucket, this makes the estimate inaccurate.
- ◇ The width of the buckets must be small enough to resolve the quantile in question: a 75 % quantile requires less buckets than a 99 % quantile (the bucket containing the latter quantile should not contain much more than 1 % of the values).

Some rules of thumb:

- ◇ Specify the minimum and maximum in such a way that typical values fall within the range, for instance with oxygen, this could be: 4 to 12 mg/l.
- ◇ Specify the width of the buckets to be at least 2 or 3 times narrower than the quantile:
- ◇ For a 95 % quantile, the width of the bucket should be at most 2 % of the whole interval, (2.5 times narrower than the 5 % that is left over). So: the number of buckets would be 50.
- ◇ For a 10 % quantile (you seek the lower range of values), the bucket width should be at most 5 %, so 20 buckets, or preferably more.

Options:

minimum:	The minimum expected value for the water quality parameter.
maximum:	The maximum expected value.
number of buckets:	The number of buckets to use
level:	The quantile level (in percents).

D.6 Percentage exceedance (*staprc*)

The *staprc* function enables you to compute the percentage of the time that a particular critical level is exceeded (for instance the concentration of bacteria must not exceed some standard) or the time that the water quality parameter is below that value (for instance oxygen should be above some standard). Besides the percentage the mean value during the time the critical level is exceeded is computed.

Options:

ccrit:	The critical level that the water quality parameter must not exceed.
above:	Indicates whether the time of exceedance is to be determined ("yes") or the time that the parameter is below the critical level ("no").

DRAFT

E User-defined wasteloads

E.1 Introduction

Occasionally a user of the WAQ water quality module needs to program wasteloads in a way that is not standard supported by the WAQ system and user interface. Examples are real-time control applications where a wasteload magnitude is made depending on the actual concentration values of substances. Another example is the combination of (multiple) intake(s) and (multiple) outlet(s), as common with power stations. This last application can then be combined with the first one if legislation would demand the switching off of outlets at higher ambient temperatures and the start-up of cooling towers.

In very early days 'user definable routines' existed that needed to be compiled and linked together with the WAQ system that came itself as a linkable library. These routines could be used for that aim. However, for some 10 years that option is not supported any more. That option is nevertheless used in-house at Deltares to implement the combination of intakes and outlets that is common for cooling water processing. We feel that we should provide the early facility again to our users, although now in a more modern way.

This appendix describes how that works and it also provides an example. The example that we provide is exactly the in-house Deltares implementation of the intake-outlet feature, but now in this new way. So, if you follow this appendix and compile the example application, then you get the standard Deltares intake-outlet feature. You may however use this as a starting point to provide your own algorithms for adjustment of intakes and outlets to run-time model outcomes.

E.2 IT-background

The background of the new way of implementation is the use of dll files, dynamic link library files. This means that the WAQ executable calls an external library that is linked at run-time. This means that the software continues to come as an executable rather than as a linkable library. It is nevertheless linking to external user routines, but now at run time. There are currently two ways known at Deltares to do this:

- 1 Through a C-language interface.
The advantage of this procedure is that if you do not need the feature, the dll also need not be present. This is the way we have implemented the "Open Processes Library" for water quality kinetics. The disadvantage is that it is difficult to use Fortran 90 derived types through the C-language interface, because they are not equivalent to C-structures. That is why we have not chosen this way for the user wasteload routine interface.
- 2 Directly by calling the dll from the Fortran executable.
The advantage is that Fortran derived types can be used as a convenient way to group all properties of a wasteload together and to define an array of those derived types. This helps you very much to keep your program simple, so this approach is selected for the user wasteload routine interface. The disadvantage of this procedure is however that the dll should always be present, because the Fortran launcher checks its presence at start-up of the executable, whether you use it or not. For this reason a dll is delivered with the sample application. This dll can always be used in case you furthermore do not use the user wasteload routine interface. If you need the user wasteload routine interface, you just replace the default dll with yours.

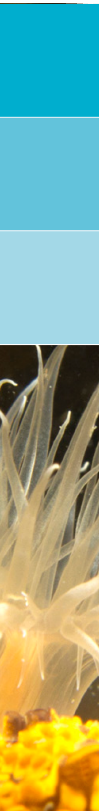
It may turn out not to be as critical as it seems, but your compiler needs to produce a compatible dll. We are using the Intel Fortran compiler. Many compilers deliver however valid dll's for interfacing.

Note: Due to rather technical issues, on Windows, the waste load module will write to a file called "fort.32", instead of the correct monitoring file. It is possible to solve this, but the required compile option must be applied to *all* components, also the components used by other parts of Delft3D. For the moment, it is necessary to check this other file for any specific messages.



E.3 The dynamic link library

The dll is called "waq_plugin_wasteload" and should contain a subroutine called "delwaq_user_wasteload" with a prescribed parameter list. This subroutine can call any subroutine that you want to use yourself. It is however for simplicity advised that you add the source of your subroutine to the "module" file that contains "delwaq_user_wasteload" subroutine. See also the example. All subroutines are contained in one and the same module file to avoid all sorts of interface statements.



E.4 `delwaq_user_wasteload` subroutine

It has 8 parameters that will be explained in more detail here:

- 1 **nowst**
This is an integer that serves input variable that should not be changed, because changing will make the behaviour of the system unpredictable. It is the number of wasteloads. It corresponds to the number of wasteloads in the user interface and it is the dimension of all wasteload-related information.
- 2 **wasteloads**
This is an array of derived types containing all wasteload information. The array is `nowst` long. Its composition will be discussed later in more detail. In this array you will change values according to your needs.
- 3 **notot**
This is an integer that serves as input variable that should not be changed, because changing will make the behaviour of the system unpredictable. It is the total number of substances in the model. It serves as dimension for all arrays with substance related properties.
- 4 **nosys**
This is an integer that serves as input variable that should not be changed, because changing will make the behaviour of the system unpredictable. It is the number of transportable substances. So `nosys` is always smaller or equal than `notot`. The first `nosys` substances move with the water. Any other substances do not. They may e.g. contain sediment that is settled at the water bottom.
- 5 **noseg**
This is an integer that serves as input variable that should not be changed, because changing will make the behaviour of the system unpredictable. It is the number of computational elements in the system. Among these elements there will be your wasteload or withdrawal element number.
- 6 **itime**
This is an integer that serves as input variable that should not be changed, because changing will make the behaviour of the system unpredictable. It is the simulation time, generally in seconds from the reference time. The reference time is given in the user interface. You can use this variable if you want to have different behaviour of your wasteload for certain time spans. Remind however that time dependent wasteloads are supported through the normal user interface. Here you are assumed to let wasteloads react on the actual model outcome of the moment (depending on the elapsed time of simulation if you wish).
- 7 **conc(notot,noseg)**
This is a real array giving the concentration values of the substances at simulation time `itime`.
It is an input variable and you should not change the value, although probably nothing will go wrong if you did, because it is a derived variable from the actual simulation variables. If you want your wasteload to be dependent on the concentration of substance `isys` in computational element `iseg`, you can check the value of `conc(isys, iseg)` for this.
- 8 **syname(notot)**
This is a character array giving the reserved names of the substances (the substance IDs). They should not be changed because changing will make the behaviour of the system unpredictable. The length of such an ID is 20 characters. If you wonder which substance number is associated with "Salinity" (e.g. to close a source for agricultural water supply if salinity is too high) then you check once in the beginning of the simulation

```
isys=find_substance('Salinity',syname)
```


and you store this `isys` value in a local variable with the `SAVE` attribute. Then you can use it to obtain `conc(isys, iseg)` during the simulation. Be aware that the number of the substance called Salinity may vary from application to application, so do NOT program a routine that assumes that Salinity is substance 2. You should also allow for a sensible error message if the substance Salinity is not available at all. If it is not available, then you have not switched it on.

E.5 "wasteload" derived type

Since Fortran 90 we are allowed to define other types than integers, real, logicals and characters. We defined the type "wasteload". Once we did so, an array of "wasteloads" can exist just like an array of reals. Our derived type "wasteload" consists of:

- ◇ **an identification called <id>**
This is also a derived type consisting of:
 - **a unique character variable called <id>**
This id is comparable with the earlier mentioned substance id. It is also 20 characters long and you can check whether this is the wasteload that you want to change by testing its `id`. The `id` of a wasteload is also mentioned in the user interface.
 - **a not-necessarily unique character called <name>**
This is a meaningful name of at most 40 characters long, which is most useful to print messages.
 - **a character value giving the <type>** Although not supported yet in all user interfaces, many wasteloads of the same type can get the same concentration value, which shortens input procedures. E.g. all "urban

run-off" type of wasteloads can have the same concentrations. This feature is not useful for you on this location.

Because the array of wasteloads is called `wasteloads`, you can retrieve the name of wasteload 8 through `wasteloads(8)%id%name`. Its id string is in `wasteloads(8)%id%id`.

◇ **a location called <loc>**

This derived type consists of a single integer called `<segr>` containing the segment number. In the future you may expect to appear also the location in world co-ordinates or longitude-latitude here and probably also an array of segment numbers if it is a distributed wasteload covering a larger area than one computational element.

If you want to know the segment number of the wasteload with id "Outfall 7", then you loop all wasteloads to check there `%id%id` string and if you found the wasteload you looked for say as wasteload number `iwst`, then you find its computational element in: `wasteloads(iwst)%loc%segrnr`.

◇ **normal real called <flow>**

This real contains the flow rate of the wasteloads in m^3/s . You may change this value as part of your programmed wasteload handling. Please be aware that in the current versions of WAQ:

- a flow of exactly 0.0 means something special (it means that the loads are considered as mass / time rather than as concentrations times the mentioned flow. If you need a zero flow, but if you do not want to set your concentration values of the wasteload to zero, then you must specify a very low flow (say $10^{-10} \text{ m}^3/\text{s}$).
- A negative flow means that water will be withdrawn from the system. If loads (see below) are exactly zero, water will be withdrawn with the current model concentration, if not, the specified concentration will be applied for the withdrawal.

◇ **an array of normal reals called <loads(nosys)>**

If the flow of a wasteload is not exactly zero, this array is interpreted as the concentration values belonging to the flow. NOTE: this will change in the future. In the future a flag will be added that indicates whether the values will be used as loads or as concentrations.

If the flow is negative and the values in `loads()` are not exact zero, then these values will be interpreted as the withdrawn concentrations. NOTE: this will change in the future. In the future a flag will be added that indicates whether withdrawals will take place with the modelled concentrations or with a prescribed concentration.

You will adapt the values in this array for your substances of interest as part of your user-programmed wasteload. Please look in the section explaining the **syname** substances names to see how you can determine which substance number is the substance you are looking for.

E.6 Utility function find_wasteload

Within the example code a function is available to find a wasteload index number with a given ID. The function is not sensitive to the case in which the ID is given. The interface of the routine is given below. The function makes use of the routine **zoekns** also included in the dll.

```
function find_wasteload( waste_id, wasteloads) result(iwst)

! function to find a wasteload on id in an array of wasteloads

character(len=*)           :: waste_id           ! wasteload id to be found
type(wasteload), pointer :: wasteloads(:) ! array of all wasteloads (structure)
integer                   :: iwst                ! on return if found wasteload number,
                                                ! otherwise zero
```

E.7 Utility function find_substance

Within the example code a function is available to find a substance index number with a given ID. The function is not sensitive to the case in which the ID is given. The interface of the routine is given below. The function makes use of the routine **zoekns** also included in the dll.

```
function find_substance( substance_id, syname) result(isys)

! function to find a substance on id

character(len=*)           :: substance_id       ! substance id to be found
character(len=20)          :: syname(:)          ! substance names
integer                   :: isys                ! on return if found substance number,
                                                ! otherwise zero
```

E.8 Recapitulation

- ◇ concentrations then you add your code to the sample code of the user programmable wasteload dll.
- ◇ You will change the `wasteloads(mywaste)%flow` and the `wasteloads(mywaste)%loads(mysubstance)` values.
- ◇ You will initially find the wasteload number you are looking for by checking the wasteload id as contained in `wasteloads(mywaste)%id%id` against the id you are looking for. You store the found value of mywaste with the 'save' attribute in a local variable for further use.
- ◇ You will initially find the substance number you are looking for by checking the substance id as contained in `syname(mysubstance)` against the id you are looking for. You store the found value of mysubstance with the 'save' attribute in a local variable for further use.
- ◇ You may also change the value of `wasteloads(mywaste)%loc%segr` and thus relocate the wasteload to a different location. Please be aware that if the waste flow or waste withdrawal are substantial and are contained in the hydrodynamics flow database, this flow is not redirected and inconsistencies may result. If you however redirect a wasteload that is not contained in the hydrodynamic database and is just only present in the water quality simulation then you will face no inconsistencies with the redirection.
- ◇ You are advised NOT to change any of the other variables and only use their information where you need it, without changing it.

E.9 Example source code `delwaq_user_inlet_outlet`

This code is added after this manual. It is not discussed per statement, but the general philosophy is explained. The program:

- ◇ Checks if a file 'inout1.dat' exists.
- ◇ If so it reads the combinations of names for inlets and outlets from this file.
- ◇ If not so it fills a 100 locations array of combinations of names INLETnn and OUTLETnn.
- ◇ It looks in the wasteload ids whether it can find any of the combinations as provided either through the file or as filled in the arrays as defaults. NOTE the use of the utility routine `find_wasteload`.
- ◇ Note that all this is done for 'ifirst' = 1, so only at first call. Once the table of matches is filled, it is stored and furthermore used every call.
- ◇ The final setting of the 'outlet' to the values of the 'inlet' is done in the tiny piece at the end.

```
subroutine delwaq_user_inlet_outlet ( nowst , wasteloads, notot , &
                                   nosys , noseg      , &
                                   itime , conc       , syname)

! routine to set the default inlet-outlet coupling

! global declarations

implicit none

! arguments declarations

integer                :: nowst                ! number of wasteloads
type(wasteload), pointer :: wasteloads(:)      ! array of all wasteloads
                                   ! (structure)

integer                :: notot                ! total number of substances
integer                :: nosys                ! number of active substances
integer                :: noseg                ! number of segments
integer                :: itime                ! system time
real                   :: conc(notot,noseg)    ! concentration array
character(len=*)       :: syname(notot)       ! substance names

! local declarations
integer, parameter     :: mxcomb = 100        ! maximum number of combinations
integer, save          :: ifirst = 1          ! initialisation indicator
integer                :: lunrep              ! report file
logical                :: l_exi              ! file exists or not
integer                :: ncomb              ! number of possible inlet outlet
                                   ! combinations
integer                :: ninout              ! actual number of inlet outlet
                                   ! combinations
character(len=20)      :: c_in               ! read buffer name inlet
character(len=20)      :: c_out              ! read buffer name outlet
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character(len=20)    :: namin(mxcomb)    ! names inlet in the possible
                                ! combinations
character(len=20)    :: namout(mxcomb)    ! names outlet in the possible
                                ! combinations
integer              :: iwin(mxcomb)      ! wasteload number inlet of the actual
                                ! combinations
integer              :: iwout(mxcomb)     ! wasteload number outlet of the actual
                                ! combinations
real                 :: flow              ! inlet flow rate
integer              :: ipin              ! wasteload number inlet
integer              :: ipout             ! wasteload number outlet
integer              :: iseg              ! inlet segment number
integer              :: iwst              ! loop counter wasteloads
integer              :: isys              ! loop counter substances
integer              :: icomb             ! loop counter combinations
integer              :: iinout            ! loop counter of inlet outlet
                                ! combinations
integer              :: i                 ! loop counter

! Save all local variables

SAVE

! test if there are inlet outlet combinations

lunrep = 32
if ( ifirst == 1 ) then
    ifirst = 0
    write(lunrep,*)
    write(lunrep,2000)

    ! if available read list of possible inlet outlet combinations

    inquire (file='inlout1.dat',exist=l_exi)
    if ( l_exi ) then
        write(lunrep,2004)
        open ( 83 , file='inlout1.dat' )
        ncomb = 0
10      continue
        read ( 83 , '(2a20)' , end = 20 ) c_in, c_out
        ncomb = ncomb + 1
        if ( ncomb .gt. mxcomb ) then
            write(lunrep,2005) mxcomb
            call srstop
        endif
        namin (ncomb) = c_in
        namout(ncomb) = c_out
        goto 10
20      continue
        close
    else

        ! construct the default list of combination INLETxx/OUTLETxx

        write(lunrep,2006)
        do i = 1 , min(mxcomb,9)
            write(namin (i),2007) i
            write(namout(i),2008) i
        enddo
        do i = 10 , min(mxcomb,99)
            write(namin (i),2009) i
            write(namout(i),2010) i
        enddo
        do i = 100 , min(mxcomb,999)
            write(namin(i),2011) i
            write(namout(i),2012) i
        enddo
    endif
endif

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    enddo
    ncomb = mxcomb
    endif

    ! check the actual list of wasteloads with the list of possible combinations

    ninout = 0
    do icomb = 1 , ncomb
        ipin = find_wasteload( namin (icomb), wasteloads)
        ipout = find_wasteload( namout (icomb), wasteloads)
        if ( ipin .gt. 0 .and. ipout .gt. 0 ) then

            ! a combination found, print and set administration

            write(lunrep,*)
            write(lunrep,2001) ipin ,wasteloads(ipin )%id%id
            write(lunrep,2002) ipout,wasteloads(ipout)%id%id
            write(lunrep,*)
            ninout = ninout + 1
            iwin(ninout) = ipin
            iwout(ninout) = ipout

        endif
    enddo
    if ( ninout == 0 ) write(lunrep,2013)
    write(lunrep,2003)

endif

! set outlet equal to inlet flow * concentration at inlet segment for all found
! combinations

do iinout = 1 , ninout
    ipin = iwin (iinout)
    ipout = iwout(iinout)
    iseg = wasteloads(ipin)%loc%segrnr
    flow = wasteloads(ipin)%flow
    wasteloads(ipout)%flow = 0.0
    do isys = 1, nosys
        wasteloads(ipout)%loads(isys) = -flow*conc(isys,iseg)
    enddo
    do isys = nosys + 1 , notot
        wasteloads(ipout)%loads(isys) = 0.0
    enddo
enddo

c
return
2000 format (' extra functionality INLET/OUTLET')
2001 format ('      waste number:',i5,' name:',a20,' (INLET) coupled to')
2002 format ('      waste number:',i5,' name:',a20,' (OUTLET)')
2003 format (' end extra functionality INLET/OUTLET')
2004 format ('      possible INLET/OUTLET combinations will be read from ', &
            'file <inloutl.dat>')
2005 format ('      error : number of combinations exceed maximum:',i4)
2006 format ('      no file <inloutl.dat> using default combinations names')
2007 format ('INLET',i1,14x)
2008 format ('OUTLET',i1,13x)
2009 format ('INLET',i2,13x)
2010 format ('OUTLET',i2,12x)
2011 format ('INLET',i3,12x)
2012 format ('OUTLET',i3,11x)
2013 format ('      no INLET/OUTLET combination found')
end subroutine delwaq_user_inlet_outlet
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