

Water quality and aquatic ecology modelling suite

D-WATER QUALITY

Deltares systems

Water Quality and Aquatic Ecology

User Manual

D-Water Quality

Versatile water quality modelling in 1D, 2D or 3D systems including physical, (bio)chemical and biological processes

User Manual

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1 A guide to this manual

1.1 Introduction

This User Manual concerns the water quality module, D-Water Quality, developed by Deltares. The manual will guide you through the mathematical and numerical framework, guide you through and explain the possibilities of the Graphical User Interface (GUI) used in the Delft3D and SOBEK suite and illustrate the basic principles of water quality modelling.

The substances and processes to be modelled with the water quality module are selected from its Processes Library. The content of the Processes Library is different for Delft3D and Sobek. This manual focuses on water quality modelling with Delft3D, but also contains a Chapter on water quality modelling with Sobek. A further integration of the contents of the Processes Library for Delft3D and Sobek is foreseen.

The Processes Library contains a comprehensive set of substances and processes, that covers a wide range of water quality parameters. In view of making the water quality module, D-Water Quality, available as open source modelling software, the Processes Library has been optimised into one coherent standard set of substances and processes for Delft3D. Usually only a part of this will be implemented in a specific water quality model. A selection can be made with Delft3D's user interface. To facilitate the quick selection of substances and processes for a specific type of model such as a model for eutrophication or a model for dissolved oxygen Deltares intends to make available predefined sets. However, the manual is equally applicable to all selections, because the operation of the water quality module in pre-processing, processing and postprocessing is exactly the same for any selection.

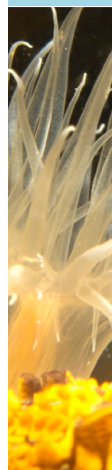
Presently, this manual does not cover all options for water quality modelling with D-Water Quality. The modelling of sediment-water interaction as based on the present standard set of processes can be included by means of a simplified approach and an advanced approach. The user interface supports only the simplified 'S1-S2' approach, for which additional substances represent two sediment layers. The comprehensive 'layered sediment' approach involves adding a sediment grid to the computational grid and including a sediment specific transport process. This can be done by manual editing of the input file that is produced by the user interface. Two additional user manuals are available for this: 'Documentation of the input file' and 'Sediment Water Interaction'. The substances and processes are the same for water and sediment in the layered sediment approach as the formulations of the processes are generic. Processes turn out differently in water and sediment depending on local conditions, such as the dissolved oxygen concentration.

To make this manual more accessible we briefly describe the contents of each chapter and appendix. If this is the first time that you will work with D-Water Quality, please refer to [section 1.2](#) to get started.

Chapter 1: A guide to this manual. The current chapter provides guidelines on how to use this manual. If you are an experienced water quality modeller you will probably need a different type of information than if this is your first encounter. Terminological conventions will help you read the manual.

Chapter 2 and chapter 3. These chapters give a brief overview of the area of application and outlines the potential the water quality model has to address a wide range of issues. Also, the place of the water quality module in the SOBEK or Delft3D suite is specified.

Chapter 4: Getting started (Delft3D) starts with the basic operation of Delft3D, explaining the Delft3D-MENU and taking a first look at the D-WAQ Graphical User Interface (GUI). File



management is briefly described.

Chapter 5: Graphical User Interface leads you in detail through the pre-processing of a water quality simulation with D-Water Quality. It describes the full functionality of the Coupling module, the Processes Library Configuration Tool (PLCT) and the WAQ-GUI.

Chapter 6: Running and post-processing (Delft3D) describes how to run a simulation, once you have defined a water quality scenario. It explains how to inspect the input and what output is generated too.

Chapter 7: Tutorials contains a worked out example of a discharge of coliform bacteria. The tutorial leads you through all the steps from the coupling to running the simulation and inspecting the results.

Chapter 8: Conceptual description explains the basic principles of water quality modelling in D-Water Quality. The explanation is focussed on the mass balances and the advection-diffusion equation.

Chapter 9: Principles of water quality modelling describes in broad outlines the principles of physical, (bio)chemical and biological processes in the natural aquatic environment. Subsequently, the chapter focuses on how these are implemented in D-Water Quality. A comprehensive description of the formulations and the input and output items of the processes can be found in Technical Reference Manual, **Detailed description of processes (D-WAQ TRM, 2013)**. Some processes developed by Deltares are not discussed in this manual. These modules can be made available upon request. As the water quality module is open source software it also has a facility to modify the formulations of existing processes or to add new substances and processes. This is described in 'Open Processes Library, User Manual'.

Some processes are not discussed in this manual either because they have not been integrated into the standard set of processes or because they are under development such as module DEB for grazers (shell fish), module MICROPHYT for microphytobenthos, and a module for aquatic macrophytes. These modules can be made available upon request.

Chapter 10: Numerical aspects. D-WAQ is a numerical model. Therefore, knowledge of the numerical aspects is needed when working with water quality models. **Chapter 10** gives you a background on numerical aspects such as (numerical) dispersion. Also, the numerical solvers that are available in D-WAQ are explained in detail.

Chapter 11: Special features gives an overview of special features like online coupling with Delft3D-FLOW, domain decomposition, coupling between Delft3D and SOBEK.

References gives a list of publications and documents referenced in this document, and a list of related publications.

Appendix A: File descriptions gives brief descriptions of input and output file types (file content and file format).

Appendix B: Standard substance files. Examples of predefined sets of substances and processes for coliform bacteria, dissolved oxygen / BOD, and suspended sediment are provided in this Appendix. They can give you a head start when you want to simulate specific issues.

Appendix C: Statistical output functions. Detailed description of various statistical output functions.

Appendix D: Command-line arguments. Some basic commands to start the WAQ-GUI and the D-Water Quality computational core.

Appendix E: User-defined wasteloads. 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.

1.2 How to use this manual

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-WAQ could be a feast of recognition for you!

Obviously, working with D-WAQ 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-WAQ involves numerically solving the so-called advection-dispersion-reaction equation. Knowledge on the principles of this equation and its implementation in D-WAQ is necessary. Numerical skills are not required as D-WAQ 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 8](#)) and the principles of water quality ([Chapter 9](#)) 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 8](#) are a good starting point as well and you will probably understand quickly the background of D-WAQ.

After that, you should start with the tutorial in [Chapter 7](#) as it will guide you through the screens and the basic functionalities of the D-WAQ framework, without overwhelming you with a lot of details and the many possibilities and alternatives D-WAQ 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-WAQ, these chapters and appendices will be your guide to further optimise your utilisation of D-WAQ.

1.3 Typographical conventions

Throughout this manual the following typographical conventions help you to distinguish between different elements of text to help you learn about the Graphical User Interface.

| 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 the Linux and UNIX environment a forward slash (/) is used instead of the backward slash (\) for PCs. |
| "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 <i>Save</i> 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. |
| [m s ⁻¹] [-] | Units are given between square brackets when used next to the formulae. Leaving them out might result in misinterpretation. |

1.4 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-WAQ 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-WAQ state variable. D-WAQ 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-WAQ 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 relation. |
| 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-WAQ 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-WAQ contains an interface to BLOOM in the form of the process D40BLO. |
| CONSBL | A process module of the Processes Library of D-WAQ to model graz- |

| | |
|-----------|---|
| | ing 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. |

1.5 Technical specifications

This version of the manual is based on the following versions of the programs:

| Program | Description | Version |
|--------------------|---|-----------|
| Delft3D-MENU | Main Delft3D program to navigate through the individual Delft3D modules | 2.05.01 |
| Delft3D WAQ-GUI | Pre-processing Graphical User Interface for D-WAQ | 3.32.00 |
| PLCT | Processes Library Configuration Tool | 5.04.00 |
| <coup203.exe> | Executable for coupling the hydrodynamic database | 2.48.09 |
| <delwaq1.exe> | Pre-processor of water quality simulation | 5.01.01 |
| <delwaq2.exe> | Executes water quality simulation | 5.01.01 |
| <proc_def.dat> and | Process definition file(s) containing the data base of | 5.01.2013 |
| <proc_def.def> | water quality processes | 060701 |

1.6 Changes with respect to previous versions

| Version | Description |
|---------|---|
| 5.00 | Sections about one-dimensional water quality modelling with hydrodynamics from SOBEK added. |
| 4.04 | section 11.4 added; Converting results of a hydrodynamic model using z -layers |
| 4.03 | section 5.3.12 , Percentile changed to Percentage. The <i>Open PLCT</i> button moved from the Far-field water quality selection window to the Tools window. |
| 4.02 | Remark added: A directory name may not contain an apostrophe ('). Remark added: A scenario name may not contain blanks (spaces). Select statistical output window redesigned. Defining horizontal dispersion in the COUP-GUI has been removed. MENU screens updated. Limitation of 4 Gb for NEFIS files added. Introduction of the Hydrodynamic coupling selection window to <i>Define input</i> for the coupling and to <i>Start</i> the coupling. In COUP-GUI and WAQ-GUI options <i>File</i> → <i>Close</i> and <i>File</i> → <i>Print</i> removed. In equation (10.33) second term in RHS: Δt^2 changed to Δt . section A.2.3 adjusted: 'metric-coordinates' should be 'metric coordinates'. section 5.3.5 : when starting from scratch, the start and stop of the simulation will be used as default for the output period, as long as you do not specify timings yourself. Appendix E (User-defined wasteloads) added. |

| Version | Description |
|---------|--|
| 4.01 | <p>Chapter 11 renamed to Chapter References. New Chapter 11 with special features added. Functionality WAQ DD (multi domains) described in Chapter 11. Functionality Online Coupling with FLOW described in Chapter 11. In Appendix A the descriptions of the monitoring area file <*.dmo>, the QUICKIN data file <*.qin> and the QUICKIN 3D data file <*.q3d> added. Appendix C added with details on the statistical output. Appendix D added with some command-line options. Bookmarks added for PDF version. Operation of <i>Change working directory</i> updated in Chapter 3. Functionality added in Section 9.6: Anticreep. Description of observation file corrected. Improved Visualisation Area in Chapter 5.</p> |
| 4.00 | <p>Improved layout of manual. Description of Graphical User Interface.</p> |

1.7 What's new?

This section gives a concise overview of new features in the D-WAQ user-interface and the manual.

This manual concerns version xxxx of D-WAQ, which is the first open source version. In this version, the processes library of D-WAQ has undergone modifications that resulted in a revised standard set of substances and processes. These modifications have been carried out to remove duplications and redundancies from the Processes Library and to integrate coherent clusters of smaller processes into larger units, which enhances the transparency of the Processes Library and reduces the risk of accidentally leaving out relevant processes in a model application. Extensions have been made as well to enlarge the modelling potential. The changes include:

- ◇ The definition of subsets of processes, called "configurations", has been removed.
- ◇ Processes which are not routinely used have been removed.
- ◇ The state variables (substances) *DetC*, *DetN*, *DetP*, *DetSi*, *OOc*, *OON*, *OOP* and *OOSi* have been replaced by *POC1*, *PON1*, *POP1*, *POC2*, *PON2*, *POP2* and *Opal*. All processes dealing with the state variables *DetC*, *DetN*, *DetP*, *DetSi*, *OOc*, *OON*, *OOP* and *OOSi* representing organic matter have been removed.
- ◇ The processes dealing with the state variables *POC1-4*, *PON1-4*, *POP1-4* and *Opal* have been extended to include the precise formulations previously used for *DetX* and *OOX*.
- ◇ All processes dealing with resuspension, burial and digging for the state variables representing the S1-S2 sediment layers have been integrated in one single process per state variable called *S12TraXXXX*, where *XXXX* equals the state variable name (substance name). This single process makes use of the supporting processes *Res_DM*, *Bur_DM* and *Dig_DM*, where DM refers to total sediment dry matter.
- ◇ The state variables (substances) *GreenS1* and *GreenS2*, representing Green algae after settling to the bed, have been removed. Green algae that settle are now instantaneously converted to detritus, just like the present practice with settling of BLOOM algae. Similarly, Diat algae that settle are now instantaneously converted to detritus.
- ◇ The state variables *DiatS1* and *DiatS2* now exclusively represent benthic algae (micro-phytobenthos), that may grow on the sediment. Settling water Diat algae are no longer converted into benthic *DiatS1* algae, while resuspending benthic *DiatS1* and *DiatS2* algae

are no longer converted into water Diat algae.

- ◇ The previous processes *Salin* and *Chloride* have been replaced by the new *Salinchlor* process.
- ◇ The process *Tau* has been renamed to *CalTau*.
- ◇ All processes previously dealing with the extinction of visible light (VL) and ultraviolet light (UV) have been integrated in two overall processes *Extinc_VLG* and *Extinc_UVG*.
- ◇ The processes calculating aggregated parameters of organic pools (e.g. POC) in water and sediment have been integrated with the overall composition processes for water and sediment *Compos*, *S1_Comp* and *S2_Comp*.
- ◇ The processes calculating aggregated settling fluxes of organic matter have been integrated with the overall aggregated settling fluxes process *Sum_Sedim*.
- ◇ A host of new state variables (substances) has been included to extend the modelling potential of D-Water Quality, particularly relevant for the modelling of sediment-water interaction modelling and greenhouse gases. This includes state variables *VIVP*, *APATP* (phosphate minerals), *SO4* (sulphate), *SUD*, *SUP* (dissolved and particulate sulphide), *POC5*, *PON5*, *POP5* (non-transportable detritus, see below), *POS1*, *POS2*, *POS3*, *POS4*, *POS5*, *DOS* (particulate and dissolved organic sulphur), *Fellpa*, *Fellpc*, *Fellld*, *FeS*, *FeS2*, *FeCO3*, *Fellld* (dissolved and particulate iron species) *TIC* (total inorganic carbon and alkalinity), *CH4* (methane). *TIC* replaces *CO2*. State variable *EnCoc* was added to represent bacterial pollutant Enterococci.
- ◇ Several new processes have been included to support the modelling of the new state variables. This includes *VIVIANITE*, *APATITE* (precipitation of phosphate), *CONSELAC* (consumption of oxygen, nitrate, iron and sulphate, and the production of methane in the mineralization of organic matter), *SPECSUD*, *OXIDSUD*, *SULPHOX*, *SPECSUDS1*, *SPECSUDS2*, *PRECSUL* (speciation, oxidation and precipitation of sulphide), *SPEC-IRON*, *IRONOX*, *IRONRED*, *PRIRON* (speciation, oxidation, reduction and precipitation of iron) *OXIDCH4*, *VOLATCH4*, *EBULCH4* (oxidation, volatilization and ebullition of methane), *SPECCARB*, *REARCO2*, *SATURCO2* (speciation and water-atmosphere exchange of dissolved inorganic carbon), and *EnCocMRT* (mortality of Enterococci).
- ◇ A new module has been included for the mortality and (re-)growth of terrestrial drowned vegetation. This concerns additional state variables *VBNN*, where *NN* is a number from 01 to 09, and *POC5*, *PON5*, *POP5*, *POS5*, into which the non-transportable detrital biomass (stems, branches, roots) is released at mortality.

Enhancements dd. January 2013 (version 4.99.29102):

- ◇ The manual has been revised in view of the revised and extended standard set of substances and processes in the Processes Library of D-Water Quality, the extension of D-Water Quality with an option for advanced sediment-water interaction, and the transition to open source D-Water Quality.
- ◇ The manual has been extended with a Chapter on water quality modelling with Sobek.

Enhancements dd. November 2006 (version 3.29.37):

- ◇ **Select statistical output** window redesigned.
- ◇ Defining horizontal dispersion in the COUP-GUI has been removed.
- ◇ Introduction of the **Hydrodynamic coupling** selection window to *Define input* for the coupling and to *Start* the coupling.
- ◇ [Section 5.3.5](#): when starting from scratch, the start and stop of the simulation will be used as default for the output period, as long as you do not specify timings yourself.
- ◇ [Appendix E \(User-defined wasteloads\)](#) added.

Enhancements dd. November 2005 (version 3.29.08):

- ◇ Detailed description of the statistical output functions
- ◇ Online coupling with Delft3D-FLOW
- ◇ Coupling in case of domain-decomposition
- ◇ Online coupling between SOBEK and D-Water Quality
- ◇ Detailed description of the balance output options

1.8 Backward compatibility

The present version of open source D-Water Quality is generally backward compatible with the previous non open source version. However, there are a few non-backward compatible items in the Processes Library. With very few exceptions older input files of existing models are still supported. The input processor delwaq1.exe makes the necessary modifications and reports them in the .lsp message file. Non-backward compatible items are printed as warnings with a reference number. These references are listed here.

- 1 void.
- 2 The concentration of detritus N, P and Si as well as OON, OOP, OOSi in the deep sediment boundary (layer "S3") are now specified directly as a solid phase concentration (FrDetNS3 in gN/gDM, FrDetPS3, FrDetSiS3, FrOONS3, FrOOPS3, FrOOSiS3). In previous versions, the carbon to X ratio was used (C-NDetCS3, C-PDetCS3, C-SDetCS3, C-NOOCS3, C-POOCS3, C-SOOCS3). If one of the latter constants has been detected in your input file, please replace by the appropriate new constant. Note: these numbers only have a meaning if the item SWDigS2 = 1.
- 3 The concentration of AAP in the deep sediment (layer "S3") is now specified directly as a solid phase concentration (FrAAPS3 in gP/gDM. In previous versions, the concentration in TIM was used (FrAAPTIMS3). If the latter constant has been detected in your input file, please replace by the new constant. Note: this number only has a meaning if the item SWDigS2 = 1.
- 4 The concentration of metals (As, Cd, Cr, Cu, Hg, Ni, Pb, Va, Zn) in the deep sediment (layer "S3") is now specified directly as a solid phase concentration (e.g. QCdDMS3 in mg/kgDM). In previous versions, this concentration was specified via the concentrations in IM1, IM2, IM3, Phyt and POC (e.g. QCdIM1S3, QCdIM2S3, QCdIM3S3, QCdPHYTS3, QCdPOCS3). If one of the latter constants has been detected in your input file, please replace by the appropriate new constant. Note: these numbers only have a meaning if the item SWDigS2 = 1.
- 5 The concentration of organic chemicals (153, Atr, BaP, Diu, Flu, HCB, HCH, Mef, OMP) in the deep sediment (layer "S3") is now specified directly as a solid phase concentration (e.g. QATrDMS3 in mg/kgDM). In previous versions, this concentration was specified via the concentrations in Phyt and POC (e.g. QATrPHYTS3, QATrPOCS3). If one of the latter constants has been detected in your input file, please replace by the appropriate new constant. Note: these numbers only have a meaning if the item SWDigS2 = 1.
- 6 Where previously up to two substances represented biogenic silica (DetSi and OOSi), the Processes Library now uses just one substance (Opal). DELWAQ will automatically convert DetSi to Opal, and neglect OOSi. Biogenic silica formed within the model domain as a result of algae mortality will be released as Opal, will dissolve and will be available for uptake by algae. A problem exists if the user has specified an inflow of biogenic silica to the model domain in the form of the substance OOSi via boundary conditions and/or waste loads. This part of the biogenic silica will no longer dissolve, will not be available for algae and will not count in the output parameter total silica (TotSi). To avoid this problem, the user has to add the boundary concentrations and waste loads of OOSi to the boundary concentrations and waste loads of DetSi or Opal.

DRAFT

2 Introduction to D-WAQ (SOBEK)

2.1 SOBEK-Rural 1DWAQ (Water Quality)

2.1.1 Introduction

General

Water quality modelling is a proven and accepted tool to support water quality management and integrated water management. It answers questions like: What are the effects of the current water management policy? What happens if we implement alternative policies? Which policy is the most effective? Etc.

SOBEK allows you to build water quality models for areas which have been modelled already in the Water Flow module of SOBEK-Rural. It offers you some interesting features to make use of experience gained by previous users of SOBEK, without taking away the flexibility to build your own tailor-made water quality model. This chapter will introduce water quality modelling with SOBEK to you. Before you start, we expect you to be familiar with SOBEK-Rural Water Flow module.

The current introduction is meant for users of both the Rural version and the River/Estuary version of SOBEK. Most of the theory presented herein can be used and understood in both model suites. On a few occasions however, we will provide specific information for either the Rural/Urban version (SOBEK-Rural/Urban) or the River/Estuary version (SOBEK-River). This will be indicated clearly.

Features SOBEK-Rural 1DWAQ (Water Quality)

- ◇ Based on the Delwaq- program, which offers you more than 20 years of collective water quality modeling experience world-wide.
- ◇ Models almost any water quality variable and its related water quality processes
- ◇ Highly flexible due to the many standard options and user-defined options available
- ◇ Uses a library of 600 processes and substances, including eutrophication, adsorption, desorption, nutrients, bacteria, oxygen, phytoplankton, heavy metals and micro-pollutants
- ◇ The interactive processes editor allows you to select the water quality variables and processes you want to model
- ◇ Pre-defined sets of water quality variables and processes can be used for particular problems or following the standard set of rules and regulations for specific regions
- ◇ To analyse the origin of pollutants in any water system, fraction computations can be easily made.
- ◇ No additional input data is required for fraction computations, which makes it easy to trace water or pollutants from to its source throughout the network
- ◇ State-of-the-art numerical schemes use a finite volume approach and display mass balances
- ◇ Fully integrated with the standard user interface, which means that standard network editing, animations, graphs and other post-processing facilities of SOBEK are used.
- ◇ Automated link to the SOBEK-Urban product lines, which allows you to view water quality in an integrated urban-rural context
- ◇ Various options are available to avoid the tedious job of defining your boundary conditions. For example defining default boundary values for clusters of inflow locations. The possibility to overwrite these defaults for specific locations, and the option to link your own ASCII input file with boundary data



What is a water quality model?

A water quality model has one or more "state variables", "pollutants" or "substances", which enter the modelled area through model boundaries or lateral inflows. They move with the currents through the modelled area. At the same time they may show their own specific behavior in the aquatic environment. This can be a simple decay, but also an interaction of transformation between different state variables.

Water quality modelling can be applied to a wide range of water quality problems. Each one of those problems requires the modelling of a specific pollutant or group of pollutants. It is often necessary to include groups of state variables, if the model equations for the individual state variables are connected to each other. For example, the decay of the state variable BOD causes the consumption of an equivalent amount of the state variable dissolved oxygen. Another example: the sedimentation of the state variable(s) representing inorganic suspended particles causes an equivalent sedimentation of the state variable adsorbed cadmium. Usually, the relevant processes are determined to a large extent by environmental conditions: the forcing functions.

| Pollution problem | State variable(s) | Important processes | Forcing functions |
|--------------------------|---|---|---|
| Bacteria pollution | Coliform bacteria | Mortality of bacteria | Solar radiation |
| Oxygen problems | BOD (biochemical oxygen demand), dissolved oxygen | Decay of BOD, consuming oxygen and reaeration (exchange of oxygen between water and atmosphere) | Water temperature, wind speed, stream-flow velocity |
| Eutrophication | Algae, inorganic nutrients (N-NH ₄ , N-NO ₃ , P-PO ₄ , Si), particulate organic matter | Growth and mortality of algae, mineralisation of particulate organic matter | Solar radiation, water temperature |
| Heavy metals | Inorganic suspended solids, heavy metal | Partitioning, sedimentation, resuspension | Streamflow velocity, wind and waves |

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

Integrated modelling of Water Flow and Water Quality

Using SOBEK to make a water quality model implies that you work in an integrated context: you use the Water Flow module and optionally the Rainfall-Runoff module of SOBEK to predict the water movement in the modelled area. Thus, you can analyze the water quality in the surface water as a function of:

- ◇ hydrological conditions;
- ◇ meteorological conditions;
- ◇ water quality on open boundaries;
- ◇ water quantity management strategies;

- ◇ discharges of pollutants.

Overview of input items

SOBEK can deal with all types of water quality problems mentioned above. The Water Quality module operates based on the schematisation already set up for the Water Flow model and the flows computed by the Water Flow model. This means that you only have to specify a limited amount of input data:

- ◇ the time frame of the computation;
- ◇ the definition of the segments;
- ◇ the concentration of all state variables on the open boundaries and in the lateral discharges;
- ◇ the initial concentrations of the state variables;
- ◇ the dispersion coefficient;
- ◇ the substance specific processes;
- ◇ forcing functions;
- ◇ information about the numerical method and the time step.

Two types of forcing functions are usually relevant: hydraulic forcing functions, and meteorological forcing functions. The hydraulic forcing functions are automatically derived from the Water Flow module. These functions are time and space dependent. They are in particular:

- ◇ the horizontal surface area (from which the Water Quality module automatically computes the water depth);
- ◇ the width of the Water Quality-segment;
- ◇ the Chézy coefficient;
- ◇ the stream flow velocity.

The following meteorological forcing functions are included in the Water Quality module:

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

These functions are time dependent.

2.1.2 About schematisations

Basic schematisation elements

The water quality module operates based on the schematisation already set up for the hydrodynamic model. Therefore, the computation of the water quality does not require any additional elements to represent the schematisation. The relevant elements are:

- ◇ branches, optionally divided in up to 4 parallel sections (SOBEK-River ONLY)
- ◇ connection nodes (SOBEK-Rural/Urban) / nodes (SOBEK-River)
- ◇ lateral flow nodes (SOBEK-Rural/Urban) / lateral discharges (SOBEK-River)
- ◇ structure nodes (SOBEK-Rural/Urban) / (compound) structures (SOBEK-River)
- ◇ boundary condition nodes (SOBEK-Rural/Urban) / nodes (SOBEK-River)
- ◇ calculation points (SOBEK-Rural/Urban) / grid points (SOBEK-River)

Remark:

- ◇ Although it is possible to work with object ID's of more than 20 characters in modules



such as Flow, the Water Quality module can only work with ID's of 20 characters or less. Because ID's can be prefixed with an 'n' when using Water Quality, any network objects used during a Water Quality simulation should have a maximum ID length of 19 characters.

Control volumes

Some of these elements have a volume: the branches and some nodes (SOBEK-Rural/Urban only). The parts of branches between 2 grid points and the nodes with a volume are called control volumes. The water quality computations are done on a grid which is based on these control volumes. Each water quality segment or Water Quality-segment coincides with one or more control volumes. The user has the liberty to make a one-to-one projection of the Water Quality-segments on the control volumes, or to aggregate several control volumes into one Water Quality-segment. A one-to-one projection yields the maximum accuracy, but also the highest number of Water Quality-segments and the longest computation time. An aggregation will speed up the computation, but may result in a loss of accuracy. SOBEK-River does not offer too many possibilities to manage the Water Quality-segments, whereas SOBEK-Rural/Urban offers efficient tools to search and find the optimum between accuracy on one hand and computational speed on the other hand.

2.1.3 Water Balance

Water balance for control volumes

The connection between the Water Flow module and the Water Quality module is through the water balance. For the benefit of the Water Quality module, the water balance is defined for two types control volumes:

- ◇ for (sub-sections of) grid cells (called reach-segments in SOBEK-River), the balance is defined by:
 - its water volume;
 - the inflow and the outflow at the calculation points;
 - optionally, 1 or more lateral discharges;
- ◇ for nodes with a water volume (SOBEK-Rural/Urban ONLY), the balance is defined by:
 - its water volume;
 - the inflow and the outflow from and to all connected reaches;
 - optionally 1 or more lateral discharges.

Water balance check

A Water Quality model is no more than a mass balance for a number of state variables. Since these state variables are all transported by the surface water, a consistent Water Quality model can only be built upon a consistent water balance: the change of the water volume of a certain segment over time, should equal the sum of the inflowing and outflowing discharges.

In SOBEK the Water Quality model derives the water balance from the Water Flow module. Therefore, the water balance is in principle always correct. Nevertheless, it is a good modelling practice to check the water balance in the Water Quality model. This can be done as follows:

- ◇ Make a simulation with one state variable.
- ◇ No decay or transformation processes are applied.
- ◇ The initial concentration is 1 everywhere.
- ◇ The boundary concentration is constant and 1 everywhere.

- ◇ The solution should be constant and 1 everywhere.

SOBEK-Rural/Urban allows you to make such a check automatically in a fraction computation. In SOBEK-River this facility is available from version 2.51 onwards: if you define the state variable "Continuity", SOBEK provides the necessary boundary conditions and initial conditions to perform the water balance check. In older versions of SOBEK-River, you can make the check manually.

If you find that the water balance check does not work out, there are a few things you can do:

- ◇ check the mass conservation of the Water Flow module, and improve it if errors are found (this is only possible in SOBEK-Rural/Urban, whereas SOBEK-River guarantees mass conservation of the Water Flow module);
- ◇ check the schematisation if you are a SOBEK-River user: segment limits must coincide with grid points, but lateral discharges should not be placed on grid points, especially not if the grid point coincides with a segment limit.

If these actions do not have the desired effect, please contact the SOBEK Helpdesk.

Fraction computations

A very important factor in water quality computations is the transport of pollutants within the channel network. The transport of pollutants determines how far the effect of individual pollution sources reaches into the network. Since the transport of pollutants is governed by the water flows, also the transport of pollutants depends on the hydrological conditions, the meteorological conditions and the applied water quantity management strategy.

Fraction computations can provide a valuable insight in the transport of pollutants in the network. In a fraction computation, you distinguish several water types which you think are important for the water quality. A water type or fraction is defined as the water originating from one or more open boundaries and/or lateral discharges. For example, in the province of Friesland the responsible authorities consider 4 types of water for the water quality management of the regional surface water network:

- ◇ water taken from the adjacent IJsselmeer lake;
- ◇ water from the polders with a sand bottom;
- ◇ water from the polders with a clay bottom;
- ◇ water from the polders with a peat bottom.

Every fraction is represented by a state variable in the Water Quality model. For all open boundaries and lateral discharges you specify which fraction it belongs to: the model makes the concentration 100 (%) for that state variable and 0 for the other state variables. A simulation run with those boundary conditions and lateral discharges will tell you how far and how strong the effect of certain groups of water sources reaches.

Evaporation

In SOBEK-Rural/Urban it is possible to make a boundary or lateral discharge of the type "Evaporation". This means that SOBEK removes the associated water flow from the evaluation of the substances mass balances. In other words: a boundary or lateral discharge of the type "Evaporation" does not cause a transport of pollutants. Consequently, a water balance check in such a case would not produce correct results! In order to check the water balance the type name "Evaporation" should temporarily be changed into something else.

Transport of pollutants around structures

In order to model correctly the transport of substances around structures, two aspects are important, especially relate to closed structures: (1) to have separate Water Quality-segments on both sides of the structure, and (2) to make the dispersion coefficient zero at the location of the structure.

In the present version of SOBEK-Rural/Urban, the modelling of the water quality around structures may present a problem. Structure nodes are situated somewhere within a reach segment. Since the smallest possible control volume for the Water Quality module is a complete reach-segment, it is not possible to separate the reach-segment parts upstream and downstream of the structure over two Water Quality-segments. The complete reach-segment is considered a mixed volume in the Water Quality module, even if the structure is closed. We expect that this problem will not be severe. It is probably only noticeable just after a structure closes or opens.

In the present version of SOBEK-River, it is very well possible to separate the grid cells upstream and downstream of the structure over two Water Quality-segments. However, to make the dispersion zero locally is only possible if a separate branch is created for the structure, since the dispersion coefficient is necessarily constant over a branch.

2.1.4 Modelling the substance specific source term

The Delwaq Processes Library

So far, we have discussed the inflow of pollutants over open boundaries and via lateral discharges and the transport of pollutants within the open channel or sewer network, governed by the water flows computed by the Water Flow module.

In many practical cases there is a significant contribution of a wide range of "other processes". They are substance-specific and they depend on the characteristics of the substance at hand. The Water Quality module includes a process library from which the user can select the appropriate processes. For details we refer to the TRM belonging to the computational core of the Water Quality module ([D-WAQ TRM, 2013](#)).

The processes library contains the joint 20 years experience of many DELWAQ users all over the world. It contains many ready-for-use processes formulations for most of the common water quality problems.

Using the Delwaq Processes Library

You have access to the processes library through 2 User Interface modules:

- ◇ for expert users: the Processes Library Configuration Tool (PLCT);
- ◇ for end-users: the Processes Library Coefficient Editor (PLCE).

The PLCT allows you to:

- ◇ select state variables;
- ◇ select processes contributing to the substance specific source term;
- ◇ select the input parameters accessible to the end-users;
- ◇ select "extra" output parameters (on top of the concentration of the state variables).

The PLCE allows you to:

- ◇ set the values of the input parameters or coefficients which are accessible to the end-users;
- ◇ manage sets of these values, by using DELWAQ default values, project default values, and by making import and export actions.

The end-users can avoid using the PLCT by using so-called "predefined sets", for example TEWOR+ (for computing the effect of storm water overflows). Thus, the end-user benefits optimally from existing experience. The expert user however, has the full flexibility to configure the processes library according to his own needs. He can create new predefined sets and modify existing ones.

SOBEK users can easily exchange predefined sets and sets of coefficient values between each others applications. They can simply exchange the associated SOBEK files: files with the extension <*.sub> and <*.0> for a predefined set and files with the extension <*.plc> for sets of coefficient values.

2.1.5 Integration options

The Water Quality-module is able to use different numerical methods to solve the governing equations. Furthermore, some sub-options exist to arrange certain details of those methods. These selections are specified in the "Integration Options" tab form. This form also takes care of the selection of the model wide dispersion coefficient.

- ◇ Click the "Integration Options" tab.
- ◇ Select the appropriate numerical method.
- ◇ Tick your choice for the three numerical sub-options.
- ◇ Provide a model-wide dispersion coefficient.

The meaning of these actions is further discussed below.

Note: The model-wide dispersion coefficient will be ADDED to the optional space-dependent dispersion coefficient you can specify in the 'Schematisation' task.



Numerical method

The user can select the numerical technique the model will use to solve the advection-diffusion equation. The details of these options are discussed in the [D-WAQ TRM \(2013\)](#). However, the selected numerical method may impose a *stability limit* on the time step. This holds for so-called *explicit* methods. If the stability criterion for an explicit method is violated, the wq simulation crashes without giving an appropriate message.

The available *explicit methods* are:

- ◇ backward in space and time
- ◇ modified 2nd order Runge Kutta
- ◇ second order Lax Wendroff
- ◇ modified Flux Corrected Transport

The stability limit is determined by the *residence time* of the Water Quality-segments: the time needed to replace their water volume by inflowing water from boundaries, lateral discharges or adjacent Water Quality-segments. In a simulation without dispersion, this criterium can be expressed as follows:

$$\Delta t \leq F \times \frac{\Delta x}{u} \quad (2.1)$$

where:

| | |
|------------|-------------------------------------|
| Δt | time step [s] |
| F | factor ranging from 0.2 to 1.0 [—] |
| Δx | length of Water Quality-segment [m] |
| u | streamflow velocity [m/s] |

This expression can not be applied to nodes with a water volume. An alternative way of expressing it is:

$$\Delta t \leq F \times \frac{Vol}{\sum Q_{in}} \quad (2.2)$$

where:

| | |
|----------|---|
| Vol | volume of Water Quality-segment [m ³] |
| Q_{in} | inflow [m ³ /s] |

The value of F depends on the explicit numerical method which is selected, but also on the simulation conditions, which are hard to quantify. Note that adding dispersion results in increasing transports, a decreasing residence time and a decreasing allowed time step.

Two *implicit* numerical methods are available which do not have a stability criterium:

1 fully implicit direct method

- ◇ very robust;
- ◇ not so accurate;
- ◇ suited for small schematisations;

2 fully implicit iterative method

- ◇ less robust;
- ◇ not so accurate;
- ◇ very effective for complicated schematisations (a lot of branches with interaction).

Note in relation to implicit methods that:

- ◇ the necessary computation time of implicit methods may be longer than that of some explicit methods;
- ◇ even if there is no *stability* limit on the time step, increasing the time step too far will influence the *accuracy*;

there may be a stability limit from the other water quality processes.

Numerical sub-options

The user can switch on or off:

| Switch | Advised use |
|--|-------------|
| allow dispersive transport where and when the flow is zero, even if the dispersion coefficient is >0 | YES |
| allow dispersive transport over open boundaries and lateral inflows, even if the dispersion coefficient is >0 | NO |
| enforce upwind transport over model boundaries, even if the selected numerical method uses another technique elsewhere | YES |

The details of these options are discussed in the [D-WAQ TRM \(2013\)](#).

2.1.6 Processes

The WQ module of SOBEK uses the so-called "Processes Library" of the computation model DELWAQ. The **Processes** tab form takes care of the selection of the appropriate configuration of the Processes Library for the problem at hand. This comes down to the selection of state variables, processes, extra output variables and process parameters. In a second step you can edit the values of the selected process parameters.

- ◇ Click the **WQ Processes** tab. The related tab form appears.
- ◇ Tick "Calculate water quality transport".
- ◇ Tick "Use predefined processes" and use the list box to select a predefined configuration of the Processes Library.
- ◇ Tick "Do not use predefined processes" and click the "Define Processes:" *Edit* button to change the configuration of the Processes Library.
- ◇ Click the "Process Coefficients:" *Edit* button to change the values of the selected process parameters.

The explanation of this part of the input starts by explaining the selection of predefined configurations of the Processes Library Followed by a section with a brief description of the main features of the Processes Library and we will explain how to set up your own configuration of the Processes Library and we explain how to edit the values of the input parameters.

If you are satisfied about a configuration of substances and processes, you may want to use this configuration in other projects as well. In this case you use the *Export* button to store your configuration with an unique name. The next time when you open the Settings module

this configuration will be available in your "Use predefined processes" list box.

2.1.6.1 Selecting a predefined configuration

In order to select a predefined configuration of the Processes Library, you can proceed in two ways follows.

Method 1

- ◇ Tick **Use predefined processes** and use the list box to select a predefined configuration of the Processes Library.

The program presents a predefined configuration, if a set of three files is available:

- 1 a file <SOBEK\FIXED\DELWAQ\name.0>,
- 2 a file <SOBEK\FIXED\DELWAQ\name.SUB>, and
- 3 a file <SOBEK\FIXED\DELWAQ\name.DES>.

The first two files are regular output files from the program ProcEdit. The last file is a one line ASCII file holding a description of the predefined configuration.

Method 2

- ◇ Tick "Do not use predefined processes" and click the "Define Processes:" *Edit* button in the "Processes" tab form.
- ◇ Wait for the PLCT to load its input files.
- ◇ Click the "File" menu in the **Water Quality** window.
- ◇ Use the "Import" option to select and load a Processes Library configuration file (a file with the extension <*.0>).
- ◇ Use the "Save" option to save the configuration file in the present case.
- ◇ Use the "Exit" option to leave the PLCT.



Note: If you follow this procedure, you can make modifications in the Processes Library configuration for the current case, without affecting the predefined configuration file.

2.1.6.2 Configuring the Processes Library

The "Processes Library"

The Processes Library includes software to model many relevant water quality processes to address the different types of water quality problems mentioned above. This generic library has been composed of dedicated software made during 20 years of WL | Delft Hydraulics' research and application projects. It is regularly updated with extended or new process formulations. The present scope of the library is the following:

- ◇ microbiological pollution;
- ◇ dissolved oxygen;
- ◇ nutrients and eutrophication (simple and complex);
- ◇ heavy metals and phosphorus sorption (simple and complex);
- ◇ organic toxic substances like pesticides and PCB's.

In the Processes Library, a process is defined as follows: it is a physical, chemical or bio-

chemical phenomenon which is responsible for (a part of) the term S, for one or more potential state variables. The actual value of its contribution to the term S is referred to as the process flux. The Processes Library consists of individual pieces of computer code (subroutines), which each represent a process.

A process is defined in terms of:

- ◇ input items (state variables, model parameters, forcing functions);
- ◇ output items;
- ◇ computed fluxes;
- ◇ effect of fluxes on state variables.

This definition is kept in a process definition file (PDF). The PDF also contains default values for the input items, if they are relevant.

Output items play a vital role. On one hand they allow the user to monitor the correct set-up of the S term. On the other hand, an output item of one process can be an input item for another one. Thus, an inter-linked set of processes can be built. An example: the process primary production has an input item light efficiency, which is computed by a separate process, which uses the light extinction coefficient, which is computed by yet another process.

An important feature of the Processes Library is the availability of alternative versions for clusters of processes. Typically, simple and more elaborate alternatives are available. Examples are the simple and more complex approaches for phytoplankton growth, sediment modelling and sorption of heavy metals. On a smaller scale, some processes feature different alternatives: the reaeration process for example features 9 alternative formulas.

Selecting processes from the Processes Library

You can set or change the configuration of the Processes Library with the help of the Processes Library Configuration Tool (PLCT).

- ◇ Tick "Do not use predefined processes" and click the "Define Processes:" *Edit* button in the **WQ Processes** tab form.

The PLCT is started, see [section 5.1](#)

Editing the selected process parameters

The values of all input parameters selected for editing can be changed by the user. The tool which offers this functionality is called Processes Library Coefficient Editor (PLCE) The parameters are presented in groups. Two types of groups exist:

- ◇ Simple lists: groups of associated process parameters which are edited in a list.
- ◇ Tables: groups of associated process parameters which are edited in a table. The table form is used if the same process parameter occurs for more than one state variable or more than one process. Examples are: the adsorption parameters for different heavy metals, or the stoichiometry parameters for different algae species.

Note: *for expert users*

The subdivision of the parameters in groups is arranged in the file
<\SOBEK***\FIXED\DELWAQ\COEFEDIT.DAT>.



The user can use two sets of default values to fall back upon:

- ◇ The "General defaults": these are the values present in the program DELWAQ, which are documented in the Technical Reference Manual of DELWAQ's Processes Library.
- ◇ The "Project defaults".

Furthermore, the user can manage sets of coefficient values outside SOBEK, through the "Import", "Export" and "Compose" options.

- ◇ Click the "Process Coefficients:" *Edit* button on the "Processes" tab form.
- ◇ Wait for the PLCE to load its input files. The **Edit Process Coefficients** window appears.
- ◇ The process parameters can be constant or time-depended. By ticking the Edit-box, time-series can be entered for the selected process parameter. The tables are also accessible with **Ctrl+T** and the menu by selecting 'Edit' - 'Table'.
- ◇ General defaults can be imported via the menu: 'File' - 'Import' - 'General defaults'.
- ◇ Click the "Available Coefficient Groups" list box to find out which groups of input parameters you can edit.
- ◇ Select the appropriate group. If the selected group is of the list type, a coefficient list appears. If the selected group is of the table type, a coefficient table appears.



Note: You have to use the "Process Coefficients" *Edit* button and leave with *OK* in order to make the changes in the Processes Library effective!!!

- ◇ Change the parameter values by typing the new value in the appropriate box.
- ◇ Save your modifications: use the menu item 'File' - 'Save'.
- ◇ Go back to the "Processes" tab form without saving the changes: use the 'escape' key.
- ◇ Restore the DELWAQ defaults: use the menu item 'File' - 'Import' - 'General Defaults'.
- ◇ Restore the project defaults: use 'File' - 'Import' - 'Project Defaults'.
- ◇ Replace the project defaults by the current parameter values: use 'File' - 'Export' - 'Project Defaults'.
- ◇ Save the current parameter values in an external file: use 'File' - 'Export'.
- ◇ Restore the parameter values from an external file: use 'File' - 'Import'.
- ◇ Restore the parameter values from different external files: use 'File' - 'Compose'.

The 'Import' and 'Export' functions allow you to communicate with external files with the extension <*.plc> (Processes Library Coefficients).

The 'Compose' option allows you to set a "primary" source file for process coefficients at the top of the window. Below, it allows you to replace the coefficients in up to 5 groups of the primary file by those in 5 different secondary files.



Note: By default there is only one coefficient group available after installing SOBEK; "Process Parameters". More coefficient groups can be distinguished by editing the file COEFEDIT.DAT in the directory <\SOBEK***\PROGRAMS\DELWAQ\FIXED\>.

It is however highly recommended NOT to edit this file. Different versions of this file can be received from Deltares.

2.1.7 Output times

Three tab forms allow you to define the output times:

- ◇ The "Chart Output" tab form: for History Results of Water Quality in the "results in charts" task (.his output).
- ◇ The "Map Output" tab form: for "results in maps" (.map output).
- ◇ The "Balance Output" tab form: for Balance Results of Water Quality in the "results in charts" task (-bal.his output) and for the Monitoring message file in the "Simulation" task (.mon output).

These forms each allow you to specify the output period and output intervals for the related output types, for example:

- ◇ Click the "Mass Balances Output" tab.

The "Mass Balances Output" tab form appears.

- ◇ Select the output interval, expressed as a multiple of the time step: the corresponding time interval can be read from the text box on the right.
- ◇ Select the output period: either accept the start and stop time of the simulation, or specify another period manually.

Note: The effective output period is always limited to the simulation period, even if you select an output period starting before or ending after the simulation period.



2.1.8 Output options

The "Output options" form allows you to create and manage restart files and to switch the mass balances output option on and off.

- ◇ Click the "Output Options" tab.
- ◇ Click the check box under "Restart data" to make the 1DWAQ module write a restart file.
- ◇ If you want a restart file: provide a file name without an extension!! (restart file name has a limited character dimension of 8)
- ◇ Push the *Edit Info* button to type comments about the restart file you are going to create.
- ◇ Use the list box as well as the *View Info* and *Delete* buttons to keep track of existing restart files and to remove the obsolete ones.
- ◇ Set the desired output locations for history and mass balances output: "write output for all segments" or "write output for monitoring stations only".
- ◇ Set the desired output variables for history and map output (see below).
- ◇ Click the check box to switch the mass balances output option on or off.
- ◇ Click the check box to switch the balance of loads output option on or off.

The options for the output variables for history and map output are:

- ◇ "state variables only": only the modelled substances will be written in the output file;
- ◇ "extra output variables only": only the variables ticked as "output" in the Processes Library Configuration Tool will be written in the output file;
- ◇ "both state variables and extra output variables": the combination of the first two options.

Note: Selecting restart files as input for the current simulation is done on the "Simulation Options" tab form.



**Warning:**

- ◇ Since the water quality module lacks the possibility to check whether or not a restart file is valid for a given simulation, we advise you to use the *Edit Info* button to register the number and the order of the state variables.

2.1.9 Schematisation

Boundary concentrations in the Fraction computation

You do not have to specify the boundary concentrations in a Fraction computation. If you do not take any action, a Fraction computation has two or three fractions:

- ◇ water from open boundaries;
- ◇ water from lateral discharges;
- ◇ "initial water" (the occurrence of this fraction depends on the selected initial conditions).

Apart from those two or three fractions, an additional fraction is created for every new fraction you defined in the **Edit User-defined objects** window.



Note: If the first 4 characters of a fraction are equal to "EVAP", the associated water flows are neglected for the computation of substances transport!! As a consequence, during a fraction calculation the fraction 'check' might no longer be equal to 1 for locations where evaporation is modelled.

Creating user-defined object types

SOBEK uses so-called user-defined object types (or UDO's) to assist the user with the task of supplying space dependent input data. In particular, the UDO's can be used to facilitate the input of 1) boundary concentrations, and 2) space dependent input parameters. They allow the user to automatically create boundary concentrations for groups of boundaries and lateral discharges rather than for individual boundaries and lateral discharges. They can also be used to automatically create space dependent model parameters for groups of control volumes rather than for individual control volumes. This makes life considerably easier for you.

A user-defined object type establishes a link between one of the basic schematisation object types and 1) a Fraction or Boundary Type, and 2) a Surface Water Type. Default SOBEK distinguishes two Boundary Types: "Flow Boundaries" and "Lateral inflows". Further Boundary Types can be created by the user. Similarly, SOBEK knows by default only one Surface Water Type: "Normal". Further Surface Water Types can be created by the user.

A UDO is characterised by its "parent type" (one of the basic schematisation object types) and a selected Boundary Type (if the parent type has a boundary) and a selected Surface Water Type (if the parent type has a water volume).

First, you have to introduce the Boundary Types and the Surface Water Types you wish to use in your model:

- ◇ Click "Edit user-defined objects" in the selection window of the "Schematisation" task: the **Edit User-Defined Objects** window appears.
- ◇ Click the *Add* button in the "Fractions" list box on the left to create a new fraction. The **Add Fraction** window appears.
- ◇ Type a name and click *OK*.

- ◇ Use the *Rename* and *Delete* buttons to edit the list of active fractions.
- ◇ Similarly, click the *Add* button in the "Surface Water Types" list box on the left to create a surface water type. The **Add Surface Water Type** window appears.
- ◇ Type a name and click *OK*.
- ◇ Use the *Rename* and *Delete* buttons to edit the list of active Surface Water Types.

Now you create user-defined object types for every relevant combination of one of the basic schematisation object types and one of the newly defined Fractions and Surface Water Types.

- ◇ Click the *Add* button in the "Node Objects" list box on the upper right to create a new User-Defined Object type. The **Edit Node Object** window appears.
- ◇ Type the name of the User-Defined object.
- ◇ Select a Fraction from the list.
- ◇ Select a Surface Water Type from the list.
- ◇ Select a "parent object type" from the list.
- ◇ Click *OK*.

Note: If the first 4 characters of a fraction are equal to "EVAP", the associated water flows are not taken into account for the computation of substances transport! As a consequence, during a fraction calculation the fraction 'check' might no longer be equal to 1 for locations where evaporation is modelled.



Note: If you have made changes related to User Defined Objects, you have to enter "Edit Model" and save the network, in order to be sure that your changes have the desired effect. See also [item 2.1.9 Linking user-defined object types to map objects](#).



Definition of Monitoring Areas

Monitoring area's are the basic spatial units for the history and balance output. They have been created for a number of reasons.

- ◇ Schematisations may be very large. If the model becomes more and more complex from the processes point of view, the mass balance output file may become very large. This can be avoided by using Monitoring Areas.
- ◇ Segment numbers change easily. The Monitoring Area however, represents the same location, independent of the water quality segment definition.
- ◇ It may be interesting to view output for an area which typically includes more than one segment. Monitoring Areas can be used to compute spatial averages over larger areas.

Monitoring Areas are defined from the **Model Data** window.

- ◇ Select an object which has a water volume.
- ◇ Click *Edit*. The **Data Edit** window appears with a "Monitoring Area" tab.
- ◇ Click the "Monitoring Area" tab: the associated form appears.
- ◇ Use the "Monitoring Area for Current Object" to make the current object a part of one of the existing Monitoring Areas. It is of course possible that an object does not belong to any Monitoring Area at all!
- ◇ Use the "Available Monitoring Areas" list and the buttons *Add New*, *Rename* and *Delete* to manage the existing Monitoring Areas. Use the *Details* button to see which other objects belong to a certain Monitoring Area.

Warning:

- ◇ If a Water Quality-segment covers more than one object with a volume, it is possible



to attribute only a part of a segment to a Monitoring Area, or even to attribute different parts of the same segment to different Monitoring Areas. The program deals with this complication as follows: a segment is included in a Monitoring Area if at least one of the objects it consists of belongs to that Monitoring Area.

Description of the task Meteorological Data

The "Meteorological Data" task takes care of the input of two additional forcing functions for the Water Quality module: solar radiation and water temperature.

You have already specified the wind data while preparing the input for the Water Flow module. The same data are passed to the Water Quality module. In order to define the other two Meteorological functions:

- ◇ Click the "Water Temperature and Solar Radiation" list box and choose between "Enter constant values" and "Daily values for selected precipitation period".
- ◇ Click the *Edit* button.

If you have selected "Edit constant values" the **Edit Temperature** window appears and afterwards a similar window to edit the Solar Radiation.

If you have selected "Daily values for selected precipitation period" the **Edit daily values for Temperature** window appears which also allows you to edit the Solar Radiation.



Warning:

- ◇ The meaning of the Solar Radiation function in the WQ module is ambiguous. In the coliform bacteria model you have to specify the total radiation, since that number affects their mortality. In the algae model you have to specify the fraction of the radiation which can be used by algae for photosynthesis. As a guideline, that fraction is about 45 % of the total radiation.

Description of the task Schematisation

The "Schematisation" task takes care of:

- ◇ the definition of the Water Quality segments;
- ◇ the input of the concentration of the state variables on the open boundaries and in the lateral discharges (boundary concentrations);
- ◇ the definition of so-called "monitoring stations": fixed output locations;
- ◇ the input of space-dependent model parameters.

The definition of the Water Quality segments comes down to specifying which control volumes or clusters of control volumes derived from the Water Flow module will be used to set up the pollutants balances. SOBEK is equipped with an automatic grid generator to create the Water Quality segments. After generating them, the user is able to modify the created Water Quality segments.

Mathematically speaking, you have to define the boundary concentrations on every open boundary and for every lateral discharge. In practice, SOBEK has a number of options to make life easy for you:

- ◇ When you start a model, the default for all boundary concentrations is zero. If you take no further action, the computation will proceed without errors, although the results will not be very significant.

- ◇ You may define Fractions or Boundary Types, representing groups of open boundaries and/or lateral discharges, for which you set the boundary concentrations group-wise.
- ◇ You have the possibility to overwrite the concentrations per Fraction or Boundary Type for individual open boundaries or lateral discharges.
- ◇ You have the possibility to derive Water Quality module state variables from measured parameters (substanc.def).
- ◇ Finally, you can add a user-defined ASCII input file which contains information that completes or even overwrites all other input. This is done in the "Settings" task.

Since the Water Quality segments can be redefined and/or changed easily, the definition of output locations is not trivial. In the 'Settings' task you can optionally define fixed locations ("monitoring stations") which will occur in the model output under the same name, regardless the lay-out of the Water Quality segments.

For the same reason it is not trivial to define space-dependent model parameters. 'Schematisation' also takes care of this SOBEK feature: you define the parameters for the objects in the flow schematisation. SOBEK automatically translates your values to the Water Quality segments, no matter their lay-out.

- ◇ Click the "Schematisation" task box: a selection window appears.

Defining and modifying the Water Quality schematisation

You can generate a Water Quality schematisation as follows:

- ◇ Click "Edit model" in the selection window.
- ◇ Click the "Edit" menu.
- ◇ Click the option "DELWAQ Segments".

The DELWAQ segments window appears.

Before pushing the *Auto* button you have to make sure you have selected the proper option for generating Water Quality segments:

- ◇ Click *Options* and *Automatic*.

There are four predefined automatic options to generate Water Quality-segments:

- ◇ "By Reach Grid": nodes with volume and individual reach-segments will become Water Quality segments;
- ◇ "By Reach Grid Stretch";
- ◇ "By Reach": reach-segments between connection nodes will be grouped into one Water Quality-segment;
- ◇ "By Reach Stretch": reach-segments between bifurcations will be grouped into one Water Quality-segment.
- ◇ Select the proper option for generating Water Quality segments.
- ◇ Click *Auto* to generate the Water Quality segments.

Besides the automatic option of generating a schematisation it is also possible for the user to generate a delwaq schematisation by hand, or edit an automatically generated network (splitting and merging of segments).

"If you want to show the numbers of the generated segments on the map".

- ◇ Click *Options* on the NETTER task bar.
- ◇ Click *Network Data*.
- ◇ Tick on "Delwaq Id" on the "Nodes" tab form.
- ◇ Tick on "Delwaq Id" on the "Links" tab form.
- ◇ Click *OK*.

If you want to join two or more Water Quality segments into one bigger Water Quality segment proceed as follows:

- ◇ Select the Water Quality segment you want to expand in the list box.
- ◇ Click on the map somewhere inside the Water Quality segment you want to add to the one selected in the list.
- ◇ Repeat this procedure as long as you want.
- ◇ Use the *Renum* button to remove empty segment numbers.

If you are satisfied with the schematisation, save it for use in the simulation:

- ◇ Click the *File* menu in the Delwaq segments window.
- ◇ Click *Save*, and *Exit*.

Edit variables for Water Quality boundary conditions

An example of the format is given below, for a model with three state variables: 'DetN', 'NH4' and 'NO3'.

```
FRACTION 'Boundary Flow'
USEFOR 'DetN' 'Total-N' - 'NH4-N' - 'NO3-N' MIN 0.0
USEFOR 'NH4' 'NH4-N'
USEFOR 'NO3' 'NO3-N'
FRACTION 'Lateral Inflow'
USEFOR 'DetN' 'Kjel-N' - 'NH4-N' MIN 0.0
USEFOR 'NH4' 'NH4-N'
USEFOR 'NO3' 'NO3-N'
```

This file specifies different substances definitions for two fractions, one of them creates a user defined list of variables consisting of 'Total-N', 'NH4-N' and 'NO3-N', and the other creates a user defined list of variables consisting of 'Kjeldahl-N', 'NH4-N' and 'NO3-N'. In both cases the result of the expression is limited to a value of zero, to avoid negative values.



Note:

- ◇ For the sake of clarity, this example shows different names of ammonium and nitrates in the user defined substances list ('NH4-N' and 'NO3-N') and in the state variables list ('NH4' and 'NO3'). This is not strictly necessary.
- ◇ The fraction names are read case-insensitive!

Editing space dependent model coefficients

The coefficients used by the Processes Library can be made space dependent. The same holds for the dispersion coefficient. You have to provide values of a space dependent coefficient for all schematisation objects which carry a water volume ("control volumes").



Note:

You do not provide values directly for the Water Quality segments. Their relation to the schematisation objects is easily changed by the user, which would lead to a loss of data if

the space dependent coefficient values would be defined at the Water Quality segment level. In stead, they are defined at the level of the schematisation objects, and converted to the Water Quality segments by the coupling program. The conversion is volume averaged for all coefficients except the dispersion coefficient, for which SOBEK uses a length-weighted average. In this respect, the "length" of a point object is computed as the square root of its horizontal surface.

It would be quite a job to provide values of a space dependent coefficient for all individual schematisation objects. SOBEK uses the different "Surface Water Types" as groups of objects for which you can enter a common value. Of course, you can override these Surface Water Type values for individual objects. Standard, SOBEK-Rural Water Quality distinguishes only one Surface Water Type: "normal". You can create additional Types by using User Defined Objects (see 'Schematisation' task).

- ◇ Click *Edit model* in the selection window.
- ◇ Click the *Edit* menu.
- ◇ Click the *Model data* option: the **Model Data** window appears.

In this window you find a list box with all objects belonging to a selected type. This is either a basic schematisation object type or a user-defined object type. You can change the selected object type at the bottom of the window.

- ◇ Select an object type: the list of objects belonging to the selected type appears.
- ◇ Select one of the objects in the list and click *Edit*: the **Data Edit for Node ...** window appears which allows you to edit the data for this object.
- ◇ Click the *Process Coefficients* tab to bring up the *Process Coefficients* tab form.

In this tab form you find a drop-down list box which shows the coefficient you are editing ("Dispersion Coefficient" in the figure) and allows you to switch to other coefficients. You also find a *Select Coefficients* button to manage the list of editable coefficients.

Below that you find room to edit an optional value to overwrite the Surface Water Type default value. At the bottom you find a list with all existing Surface Water Types and the default values for the current coefficient.

- ◇ Fill out the list of parameter values for the Surface Water Types at the bottom.
- ◇ Optionally: specify a value for the current object overwriting the Surface Water Type default value. You can switch back to the Type default by ticking the "Use default" switch.
- ◇ Click the *Select Coefficients* button to enter a separate window to manage the list of editable coefficients.

In this window you find the "gross list" of existing process coefficients on the left side, and the list of coefficients selected for space dependent editing on the right side. The "Activated" switch refers to the space dependent parameter being used in the current simulation. It allows you to keep a set of values you have typed for later use, without actually using them in the current simulation. You can use this feature to quickly compare simulations with and without the use of space dependency for a given coefficient.

The gross list is structured with the help of coefficient groups (the same as in the Processes Library Coefficient Editor in the 'Settings' task). Within a group the coefficients are ordered alphabetically. One additional group with one coefficient is available here: the dispersion coefficient.

- ◇ Select a coefficient group at the upper left corner.

- ◇ Select a coefficient in the list box on the left.
- ◇ Move it to the list of Coefficients Selected for space dependent editing on the right by using the \gg button.
- ◇ Decide if you want the space dependent parameters to be active in the current simulation and tick the "Activated" switches accordingly.
- ◇ Delete items from the Selected Coefficients list by using the \ll button.
- ◇ Click the *Edit Coefficients* button to return to editing mode.



Note: There is no direct relation between the selection and editing of "Editable" coefficients in the 'Settings' task and the selection and editing of space dependent coefficients here. The Water Quality simulation model will evaluate both parts of its input and it will treat Activated space dependent coefficients from the 'Schematisation' task with preference over constant coefficient values from the 'Settings' task.







Note: The space-dependent dispersion coefficient will be ADDED to the model wide dispersion coefficient you can specify in the 'Settings' task.

Linking user-defined object types to map objects

Once you have created UDO's, you have to indicate which individual schematisation objects on the map belong to the user-defined object types. Proceed as follows:

- ◇ Click the button *Edit Network* of the similar menu.

In this example two new user defined objects are available: 'Type 48 Sewer overflow' en 'Type 49 Upstream boundary'. In the network two existing objects will be replaced by these two new nodes.

- ◇ Click the new object type: .
- ◇ Click the button *Set node type* of the menu 'Node': .
- ◇ Click the node with lateral inflow, that you want to change into the new object type.
- ◇ Click the object type: .
- ◇ Click the button *Set node type* of the menu 'Node': .
- ◇ Click the boundary node that you want to change into the new object type.



Note: Use the Zoom option to visualize the nodes you are modifying.



Note: You can always check your network and the actions you have done by asking Node Info.

To get Node Info proceed as follows:

- ◇ Make sure the "Edit" "Network" option is not ticked.
- ◇ Click on the node for which you want information.
- ◇ Click the Right mouse button and select "Info".

Make sure that you Save the network after editing it:

- ◇ Click the "File" menu.
- ◇ Click the option "Save > Network".

Warning:

- ◇ If you delete a user-defined object type the objects you have linked to that particular object type will not be automatically reset to the corresponding basic schematisation object type. You will have to do that manually.

Setting spatially dependant parameters and dispersion

In SOBEK it is possible to create locally dependant parameters and dispersion. The easiest way is to create a special network object, a so called Surface water type. This makes it easier to identify and edit spatially dependant parameters

Take the following steps:

- 1 Create a Surface water type in the schematisation task block, edit user defined objects:
- 2 Go to edit network and apply the newly created branch object
- 3 Right mouse-click the branch object, edit model to edit the parameters

Create a new surface water type

In **Edit User Defined Object**, create a new branch object:

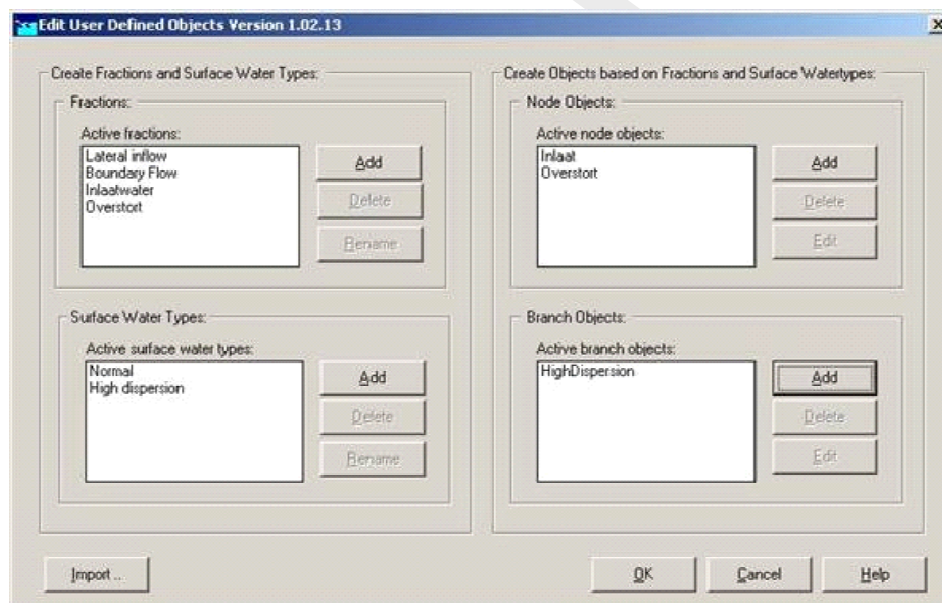


Figure 2.1: Edit User Defined Object window

First, add a new Active surface water type, then add a new branch object and link this the object to the new Surface water type:

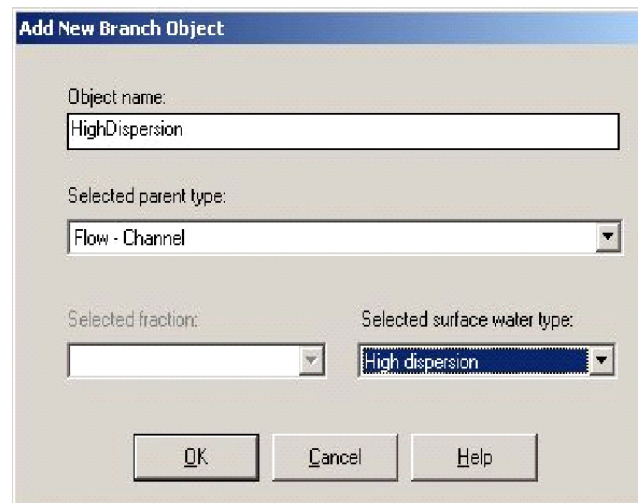


Figure 2.2: Add New Branch Object window

Edit network

Next, open Netter to edit the network. A new channel flow object is available:

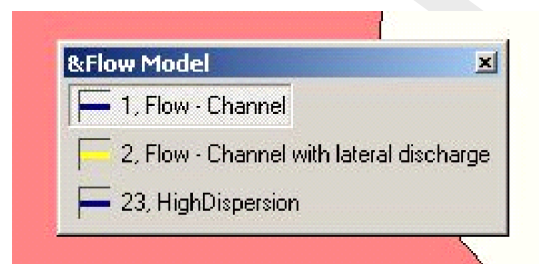


Figure 2.3: Flow Model window

Select this object and apply it.

Select a branch and right mouse-click to "edit model" and go to the tab "WQ Parameters":

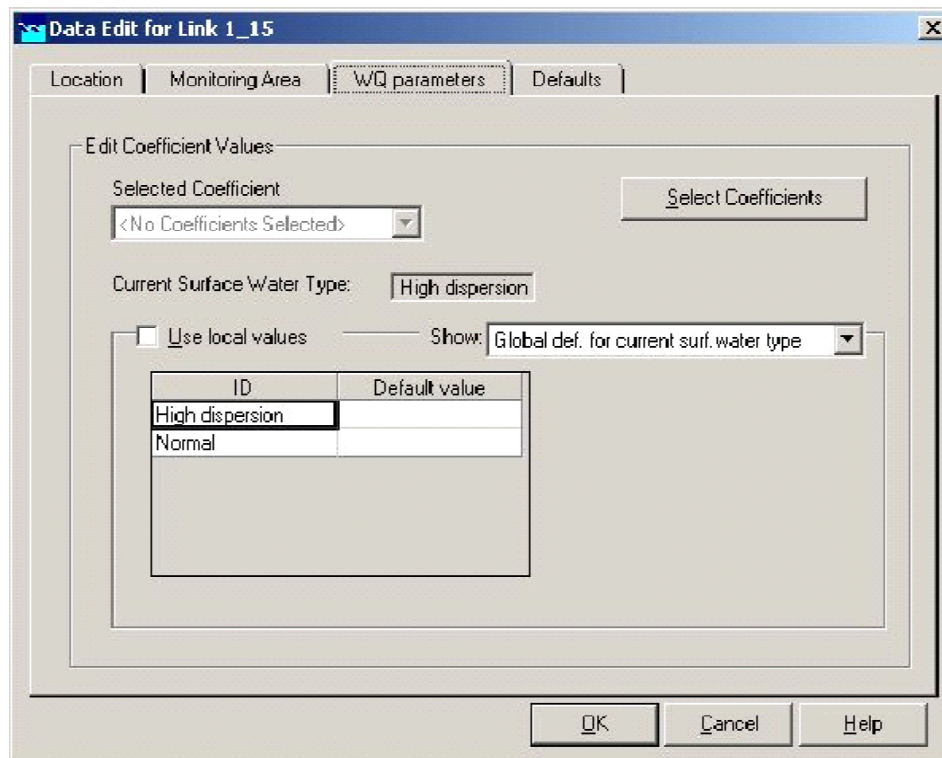


Figure 2.4: *Data Edit for Link* window, WQ Parameters tab, Edit Coefficient Values No coefficients selected.

First, click the select coefficients button. Now you can select the desired parameters. A user can define initial conditions, dispersion coefficients and process parameters by using the drop down box. Move the selected parameters to the right screen:

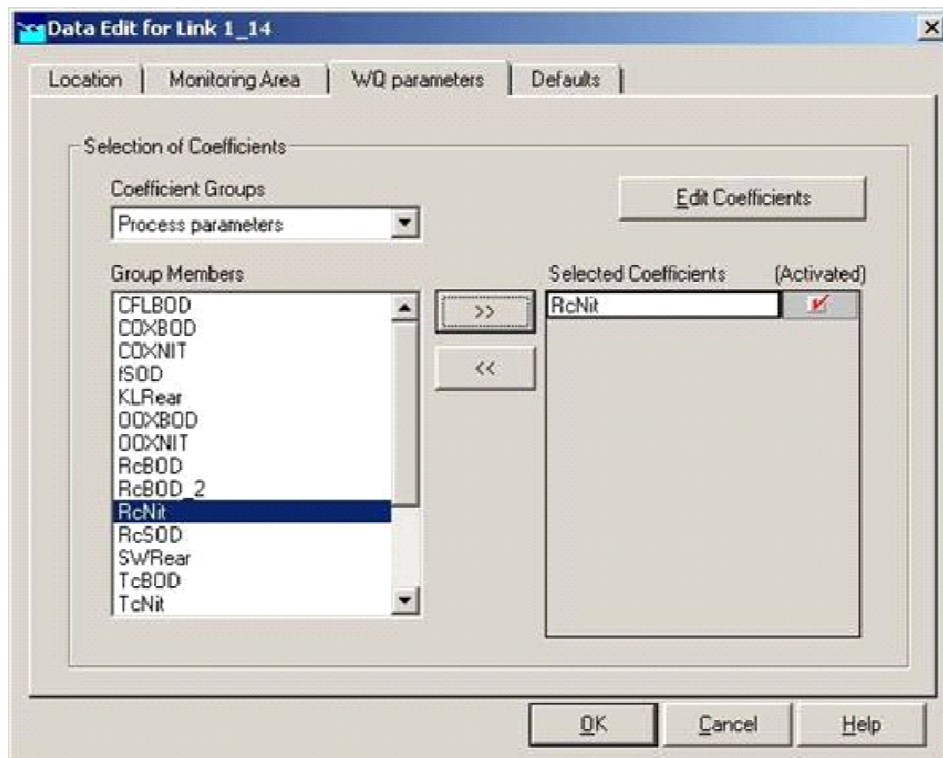


Figure 2.5: *Data Edit for Link* window, WQ Parameters tab, Selection of Coefficients, selected coefficient group is "Process parameters"

Next, select the edit coefficients button to enter the values for the parameters.

Spatially dependent parameters will be attached to surface water types of individual branch id's. To use an individual id, select the "use local value" option.

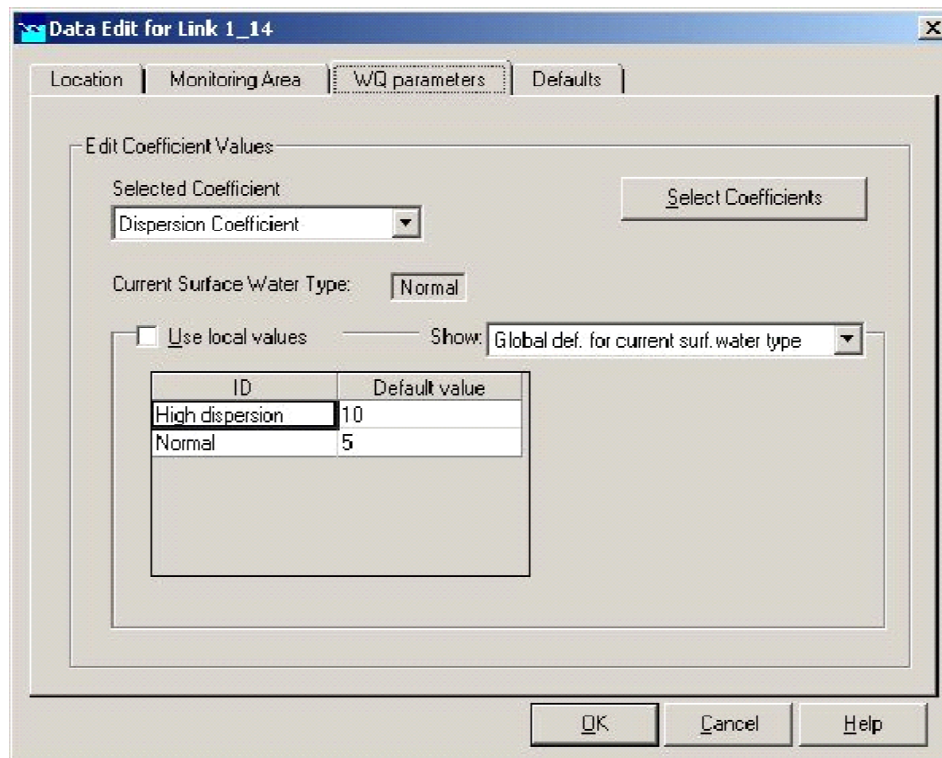


Figure 2.6: *Data Edit for Link* window, WQ Parameters tab, Edit Coefficient Values, selected coefficient "Dispersion Coefficient"

Note:

There are three levels of parameters:

- ◇ Global, set in the Settings Taskblock
- ◇ Locally by surface water type, overwrites the global value
- ◇ Locally by branch id, overwrites both global value and surface water type value.

The definition of water quality boundary concentrations

Contrary to the Fraction computations, you have to specify the boundary concentrations explicitly in Water Quality computations.

- ◇ Click "Edit model" in the selection window.
- ◇ Click the "Edit" menu.
- ◇ Click the "Model data" option: the **Model Data** window appears.

In this window you find a list box with all objects belonging to a selected type. This is either a basic schematisation object type or a user-defined object type. You can change the selected object type at the bottom of the window.

- ◇ Select an object type: the list of objects belonging to the selected type appears.
- ◇ Select one of the objects in the list and click *Edit*: the **Data Edit for Node ...** window appears which allows you to edit the data for this object.
- ◇ Click the "Water Quality" tab to bring up the "Water Quality" tab form.

Note: this tab is inactive when no DELWAQ schematisation is available for the selected object.

This is a complex window which has the following characteristics:

- ◇ A "Show" list box to switch between "global definition for this fraction" (the boundary type) and "local definition for current object" (individual object values). For both items values can be defined.
- ◇ With help of the "use local value" tick box the user can select which data are used (global or local).
- ◇ A set of options to switch between "Constant Concentrations" and "Time Dependent Concentrations".
- ◇ Click "Time Dependent Concentrations" to enter time dependent data. The layout of the window changes again.
- ◇ With help of the *Add Row*, *Insert Row* and *Delete Row* it is possible to manage the number of timesteps/rows in the list.
- ◇ With help of the *Import Table* and *Export Table* the user is able to export and import ASCII database files <*.prn> with the following file format:

```
* CONCENTRATION C1 EColi TColi OXY CBOD5
"2001-01-31;00:00:00" 20 5000 10000 5.5 1.2
"2001-02-01;00:00:00" 20 5000 10000 5.5 1.2
"2001-02-02;00:00:00" 20 5000 10000 5.5 1.2
```



Note:

If the first 4 characters of a fraction are equal to "EVAP", the associated water flows are neglected for the computation of substances transport!! As a consequence, during a fraction calculation the fraction 'check' might no longer be equal to 1 for locations where evaporation is modelled.



Note:

The substance list in this tab page corresponds with the SOBEK-WQ state variables as defined by the user. However, if the user has defined some transformation rules these variables are overruled by the ones defined by the user.

2.1.10 Use substances aliases when defining WQ boundary conditions

The list of state variables used in complex water quality models often not completely matches the list of monitored variables. This goes for example for organic nitrogen and algae biomass. Some of these state variables can easily be derived from monitored variables. Organic nitrogen can be calculated from the measured total nitrogen and/or Kjeldahl nitrogen value and the ammonium and nitrate concentrations. Algae biomass can be determined by means of the measured chlorophyll concentration. SOBEK is able to transform monitored variables into state variables via user defined computation rules¹.

Methodology

Computation rules for transformation of monitored variables into state variables can be defined by the user in the file <substanc.def>. This ASCII file is empty by default. It is accessible via the option "edit variables for WQ boundary conditions under the schematisation task block. It should be created *before* starting the input of the boundary conditions. The User Interface module responsible for the input of the boundary conditions uses the information in <substanc.def>. It checks if a transformation has to be applied for a certain boundary or lateral discharge object. If that is the case, the UI uses the transformation rules to derive a *user defined substances list* which replaces the list of SOBEK-WQ state variables in the input menu.

¹This functionality was formerly known as the "substanc.def functionality" in older versions of Deltares' water quality modelling software.

The transformation from an arbitrary set of input variables to the SOBEK-WQ state variables needs to be defined exactly by the user. This definition is subject to the following conditions:

- ◇ A SOBEK-WQ state variable needs to be expressed in a so-called *complex substance alias*, which consists of:
 - an arbitrary amount of user defined variables;
 - an arbitrary amount of real numbers;
 - using the arithmetic symbols "+", "-", "/" and "**".
- ◇ It is possible to limit the result of an expression to a certain minimum or maximum value.
- ◇ SOBEK-WQ state variables that are left out are given values of "zero" after the transformation.
- ◇ The ensemble of all substance aliases, also called a *substance definition*, may be defined separately for every fraction in the WQ model.
- ◇ If no substance definition is defined for a certain fraction, no transformation is applied for the boundary objects belonging to this particular fraction.

Format of the new <substanc.def> file

An example of the format is given below, for a model with three state variables: 'DetN', 'NH4' and 'NO3'.

```
FRACTION 'Boundary Flow'
USEFOR 'DetN' 'Total-N' - 'NH4-N' - 'NO3-N' MIN 0.0
USEFOR 'NH4' 'NH4-N'
USEFOR 'NO3' 'NO3-N'
FRACTION 'Lateral Inflow'
USEFOR 'DetN' 'Kjel-N' - 'NH4-N' MIN 0.0
USEFOR 'NH4' 'NH4-N'
USEFOR 'NO3' 'NO3-N'
```

This file specifies different *substances definitions* for two fractions, one of them creates a user defined list of variables consisting of 'Total-N', 'NH4-N' and 'NO3-N', and the other creates a user defined list of variables consisting of 'Kjel-N', 'NH4-N' and 'NO3-N'. In both cases the result of the expression is limited to a value of zero, to avoid negative values.

Note:



- ◇ For the sake of clarity, this example shows different names of ammonium and nitrates in the user defined substances list ('NH4-N' and 'NO3-N') and in the state variables list ('NH4' and 'NO3'). This is not strictly necessary.
- ◇ The fraction names are read *case-insensitive*!
- ◇ Use space between the substances, the arithmetic symbols "+", "-", "/" and "**" and the numbers!

Practical aspects

It will happen many times that either the list of SOBEK-WQ state variables changes or the transformation rules change during the course of a project. If boundary conditions have been defined already, some boundary conditions data may become meaningless. The User Interface treats such cases as follows: it reads all values which have been put in before, but maintains only those which have a meaning. If the user saves the data, all meaningless data are lost.

A boundary condition for a state variable computed by a complex substance alias becomes a *missing value* if at least one of the user defined variables in the substance alias represents a

missing value.

The computational core uses the information in the <substanc.def> file to translate the boundary conditions for the user defined variables to the boundary conditions for the list of SOBEK-WQ state variables. However, the computational core does not read this information directly from the <substanc.def> file. The User Interface copies the relevant *substance definition* before every block of boundary conditions data in the files <boundwq.typ> (fraction) or <boundwq.dat> (object). These two files are then passed on to the computational core. If the user changes the <substanc.def> file, he or she has to start the boundary conditions UI module to copy the changes to <boundwq.typ> and <boundwq.dat>. It is advised to enter all objects or boundary types for which the *substance definition* has been changed and explicitly save the data, to make sure that the changes have become effective.

In relation to the previous aspect, expert users should take care while supplying ready made <boundwq.typ> and <boundwq.dat> files to SOBEK. If they contain *substance definitions* (necessary to make the computational core run) the user should be aware of the fact that these will be replaced by the ones in <substanc.def> as soon as the UI is activated.



Remark:

- ◇ This functionality was formerly known as the "substanc.def functionality" in older versions of Deltares' water quality modelling software.

User defined boundary conditions

Complex water quality models often use a set of state variables which does not match the list of monitored variables. SOBEK is able to perform the transformation of an arbitrary set of water quality variables to SOBEK-Rural Water Quality state variables. This transformation needs to be defined exactly by the user. The total of all substance definitions is stored in a file called <substanc.def>. This file is accessible by an ASCII editor through one of the buttons under the "Schematisation" task box. This file is empty by default. It should be created before starting the input of the boundary conditions.

The User Interface module responsible for the input of the boundary conditions uses the information in <substanc.def>. It checks if a transformation has to be applied for a certain boundary or lateral discharge object. If that is the case, the UI uses the transformation rules to derive a user defined substances list which replaces the list of SOBEK-Rural Water Quality state variables in the input menu.

2.1.11 Simulation

Description of the task

After you have finished the input tasks, you can try to run the model.

- ◇ Double-click the "Simulation" task. Rainfall-Runoff models (optional), Emission models (optional) and the Water Flow module (necessary) will first run: they will compute the necessary flow data for the Water Quality module.

The second time you run the "Simulation" task, it may not be necessary to rerun the Rainfall-Runoff, Emission and the Water Flow modules. This is the case if you have not changed anything in the input for these modules. SOBEK detects that there is output from the Water Flop module available and asks you whether you want to use this output.

The WQ model run consists of the following steps (you will see windows opening and closing

for each of these steps):

- ◇ Pre-processing (preparation of simulation);
- ◇ Quantity to Quality (conversion of output from CF module, preparation of boundary conditions for Fraction computation);
- ◇ DELWAQ1 (reading and checking of input for WQ module, and processing the configuration of the Processes Library for extra water quality processes; is skipped in case of fraction computations and when the "processes active" switch has been disabled (Settings module);
- ◇ DELBEL (if balance of loads output option is activated in Settings module)
- ◇ DELWAQ2 (performing the simulation);
- ◇ Postprocessing (conversion of output, in particular mass balances output).

You may want to check the simulation messages, especially if an error occurs.

- ◇ Click the right mouse button while it is positioned in the "Simulation" task box.
- ◇ Click "Simulation Messages". The **Simulation Messages** window appears.
- ◇ Select the appropriate messages file and click the *View* button.

The available files are:

- ◇ Pre-processing;
- ◇ List file of pre-processing: output from DELWAQ1 (<*.lst> and <*.lsp> files);
- ◇ List file of loads computation: output from DELBEL (<*.lst> file);
- ◇ Monitoring file: output from DELWAQ2 (<*.mon> file).

2.1.12 Results in maps

Description of the task

- ◇ Double-click the "Results in maps" task box. The NETTER programme is started
- ◇ After \File\Open, the **Select item** window appears.
- ◇ Select the appropriate output file and click the *OK* button, or double click on the output file name description itself.

The available water quality output files are:

- ◇ Map Results of Water Quality: regular output from DELWAQ, consisting of the state variables and/or the other selected output parameters (as defined within the Settings module);
- ◇ Balance of Loads: regular output file from DELBEL, consisting the waste loads over the boundaries per state variable.

DRAFT

3 Introduction to D-WAQ (Delft3D)

Deltares has developed a unique, fully integrated computer software suite for a multi-disciplinary approach and multi-dimensional computations for oceanic, marine, coastal, estuarine and river areas. It can carry out simulations of flows, sediment transport, waves, morphological developments, water quality and ecology. It has been designed for experts and non-experts alike. The Delft3D and SOBEK suite are composed of several modules, grouped around a mutual interface, while being capable to interact with each other. D-Water Quality, the subject of this manual, is one of these modules.

3.1 Areas of application

D-WAQ is a multi-dimensional water quality model framework. It solves the advection-diffusion-reaction equation on a predefined computational grid and for a wide range of model substances. D-WAQ allows great flexibility in the substances to be modelled, as well as in the processes to be considered. D-WAQ is not a hydrodynamic model, so information on flow fields is derived from Delft3D-FLOW or SOBEK ([Delft3D-FLOW UM, 2013](#); [SOBEK UM, 2013](#)), although any description of the movement of water would be suitable if available in the right format.

A wide range of model substances is available in D-WAQ including:

- ◇ conservative substances (salinity, chloride, continuity and up to five tracers)
- ◇ degradable substances (up to five degradable tracers)
- ◇ suspended sediment (up to three fractions)
- ◇ temperature
- ◇ nutrients (ammonia, nitrate, phosphate, adsorbed P, vivianite-P, apatite-P, silicate, opal)
- ◇ organic matter (subdivided in carbon, nitrogen, phosphorus and sulphur components)
- ◇ dissolved oxygen
- ◇ inorganic sulphur components (sulphate, sulphide)
- ◇ iron components (up to 7 oxidized and reduced dissolved and particulate components)
- ◇ methane
- ◇ total dissolved inorganic carbon (carbon dioxide)
- ◇ BOD and COD (respectively Biological and Chemical Oxygen Demand)
- ◇ phytoplankton biomass (algae species)
- ◇ microphytobenthos biomass (benthic diatoms)
- ◇ grazers biomass (modelled as forcing function)
- ◇ terrestrial vegetation biomass (drowned vegetation)
- ◇ bacterial pollutants (4 species)
- ◇ heavy metals
- ◇ organic micro-pollutants

D-WAQ allows you to specify an even wider range of physical, (bio)chemical and biological processes. The processes are stored in the so-called Process Library from which any subset of substances and processes can be selected. Examples of the processes included are:

- ◇ settling (sedimentation) and resuspension
- ◇ reaeration of oxygen
- ◇ algae growth and mortality
- ◇ mineralization of organic matter
- ◇ (de)nitrification
- ◇ phosphate adsorption and precipitation
- ◇ partitioning (adsorption, precipitation) of heavy metals
- ◇ partitioning, degradation and volatilization of organic micro-pollutants



- ◇ mortality of bacterial pollutants

D-WAQ has a wide applicability. Basically, it can be used whenever any (combination) of the substances mentioned above is of interest. The only requirement is the availability of a hydrodynamic description of the water system. For example, D-WAQ has been applied for studying:

- ◇ eutrophication of lakes, reservoirs, estuaries and seas with or without sediment diagenesis
- ◇ dissolved oxygen depletion in stratified systems
- ◇ impact of a sewage outfall on nutrient concentrations and primary production
- ◇ transport of heavy metals through an estuary
- ◇ accumulation of organic micro-pollutants in fresh water basins
- ◇ the emission of greenhouse gases from reservoirs
- ◇ sediment transport
- ◇ water temperature as related to outfalls
- ◇ etc.

Not all options are GUI-PLCT supported, the option for advanced 'layered sediment' modelling in particular, but additional manuals are available for application. Moreover, some processes developed by Deltares are not discussed in this manual because they have not been integrated into the standard set of processes. This concerns the simplified pH process pH_SIMP, the advanced module DEB for grazers (shell fish), the advanced module MICROPHYT for microphytobenthos, and the module for aquatic macrophytes (the biological modules are under development). These modules can be made available upon request.

3.2 Coupling to other modules

D-WAQ makes use of the hydrodynamic conditions (velocities, water elevations, density, salinity, vertical eddy viscosity and vertical eddy diffusivity) calculated in the Delft3D-FLOW or SOBEK module. In combination with Delft3D-FLOW also wave characteristics (wave height, wave length and wave period), which are be important in sedimentation-erosion studies in relatively shallow areas, can be derived from the Delft3D-WAVE module ([WAVE UM, 2013](#)).

3.3 Utilities

For using D-WAQ the following utilities are important:

| | |
|---------------------|---|
| QUICKIN | for preparing and manipulating grid oriented data, such initial conditions or spatially varying process parameters or forcing functions. See manual QUICKIN UM (2013) |
| D-Waq DIDO or WQINT | for horizontally aggregating the hydrodynamic result in order to reduce computation time. See manual DIDO UM (2013) |
| D-Waq PLCT | for selecting the substances needed for the water quality model. |
| GPP | for visualisation and animation of simulation results. See manual GPP UM (2013) |
| Delft3D-QUICKPLOT | another tool for visualisation and animation of simulation results. See manual QUICKPLOT UM (2013) |

For details on using these utility programs you are referred to the respective User Manual.

4 Getting started (Delft3D)

4.1 Starting Delft3D

The Delft3D suite is a range of modules that can be run independently of one another. The main menu of Delft3D provides access to each of the main modules. Delft3D-MENU can be started either:

- ◇ In Microsoft®Windows, select Delft3D in the Programs Menu or click on the Delft3D icon on the desk-top
- ◇ In Linux/UNIX, type `delft3d-menu` on the command line.

Next the title window of Delft3D is displayed, [Figure 4.1](#):

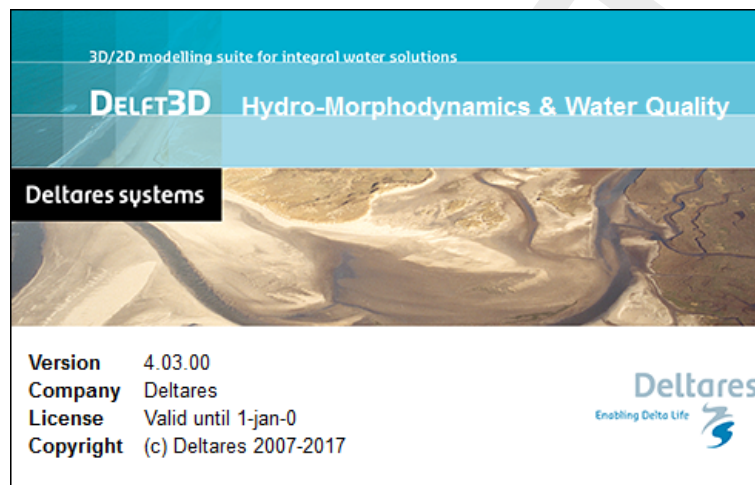


Figure 4.1: Title window of Delft3D

After a short while the main window of the Delft3D-MENU appears, [Figure 4.2](#).

Whether or not you may use specific Delft3D modules and features depends on the license file you have (`delft3d_hostid.lic` in your `DS_Flex` directory).

There are two ways to exit the Delft3D-MENU:

- ◇ Click *Exit*.
- ◇ Click the 'close' button (×) in the top-right corner of the menu bar.

4.2 Water Quality module

The water quality selection window is opened by selecting *Water Quality* in the main menu. The **Far-field water quality** selection window is shown in [Figure 4.3](#).

The **Water quality (WAQ)** window shows the steps that you have to take one by one to undertake a water quality simulation. The steps can be subdivided in pre-processing (*Coupling, Processes, Define input*), processing (*Waq (1), Waq (2)*), post-processing (*Reports, GPP, QUICKPLOT*) and additional tools (*Tools*).

The steps are briefly described below and will be dealt with in more detail in the next chapters.

Processes Activates the Processes Library Configuration Tool (PLCT)

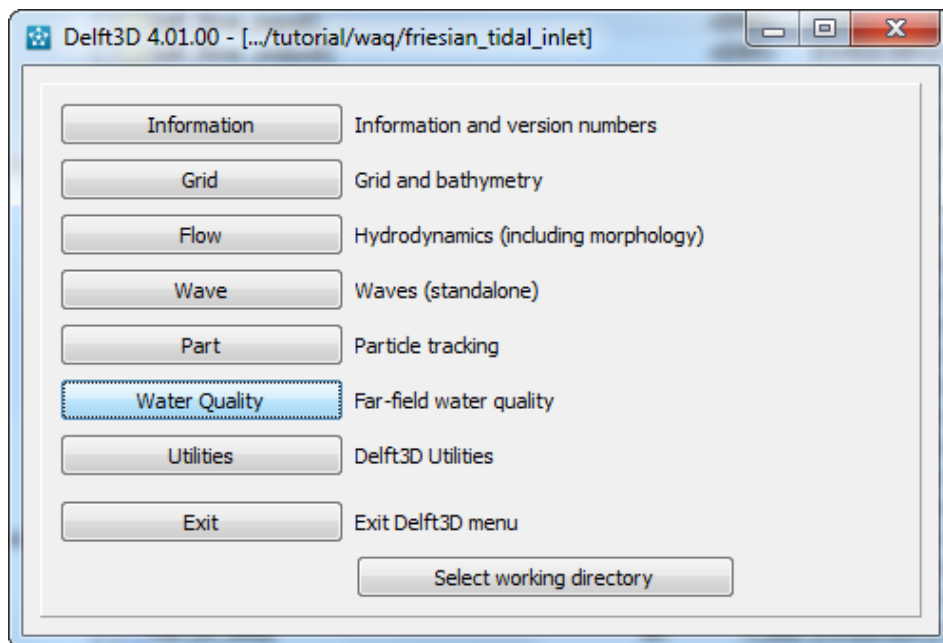


Figure 4.2: Main window of Delft3D-MENU

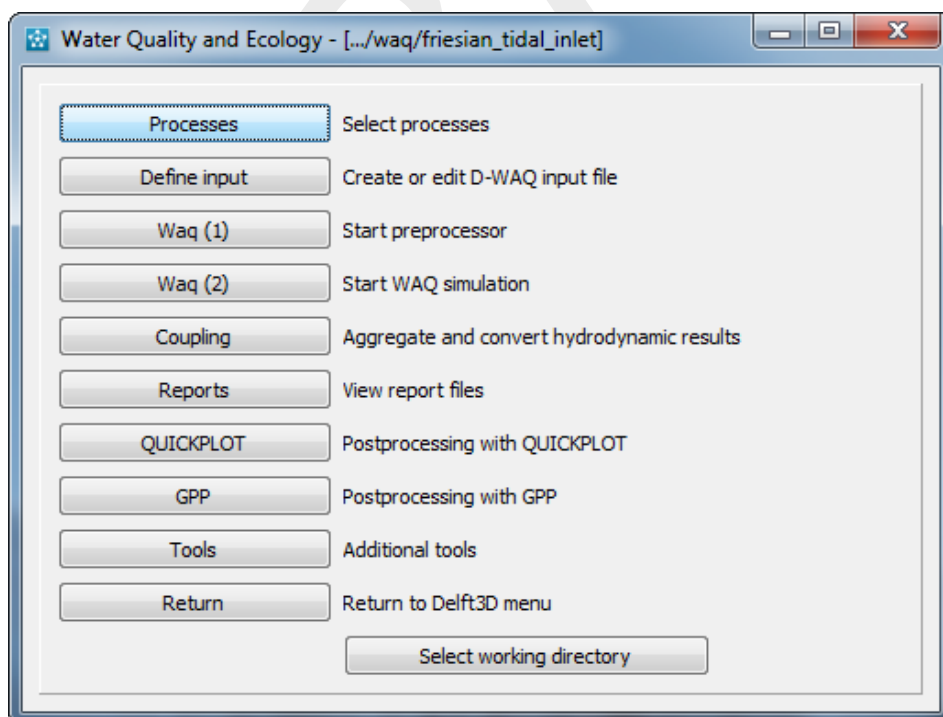


Figure 4.3: Selection window for **Water quality**

| | |
|---------------------|--|
| | With the PLCT you can select the state variables and water quality processes you want to include in the simulation. |
| <i>Define input</i> | Create or edit input file The Graphical User Interface (GUI) is started in which you can define the input for a water quality computation. The information will be stored in a scenario <*.scn> file and an input file (<*.inp>). |
| <i>Waq (1)</i> | Run pre-processors Two pre-processors will check the input file for errors and activate the user-defined water quality processes. The pre-processing will create a <*.lst> and a <*.lsp> file which you can check under the <i>Reports</i> menu item. |
| <i>Waq (2)</i> | Run D-WAQ model The water quality simulation is started. The model will create binary output files (<*.map>, <*.ada>, <*.his>, <*.hda> and <*.bal>) which can be visualised with the GPP and QUICKPLOT packages and an ASCII output file (<*.mon>) which can be inspected under the <i>Reports</i> menu item. |
| <i>Coupling</i> | Convert and/or aggregate Hydrodynamic results. D-Water Quality uses the grid layout and the results from a hydrodynamic calculation in a particular form. The output files from the model that provides these results may or may not fit the form D-Water Quality expects. If not, a separate coupling step is required. Note: however, that with recent versions of Delft3D-FLOW this step is no longer needed, as the relevant files are written directly by Delft3D-FLOW (see section 5.2). |
| <i>Reports</i> | View report files This option allows you to inspect the ASCII report files generated by D-Water Quality. |
| <i>GPP</i> | Post-processing with GPP Starts the GPP visualisation package. |
| <i>QUICKPLOT</i> | Post-processing with Delft3D-QUICKPLOT Starts the QUICKPLOT visualisation package. |
| <i>Tools</i> | Additional tools Configure your own Processes Library using the Open PLCT. Boundary conditions for a certain model domain can be derived from a larger model domain. This so-called nesting can be performed under <i>Tools</i> . |

**Remark:**

- ◇ It is possible to skip steps, if certain information is already available. For example, if you already have assembled the substances and water quality processes in a so-called substances file (via the *Processes* step, you can skip that step, similarly for the *Coupling* step.. The menu works completely modular and modules can be run independently in any order.



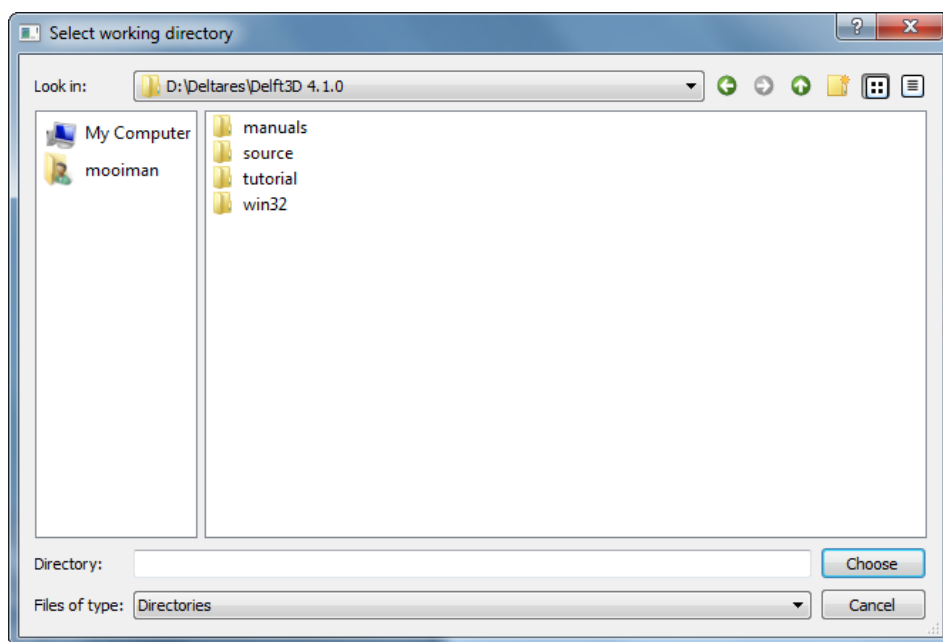


Figure 4.4: Select working directory window

4.3 Select working directory

It is possible to select and/or change the default working directory in which the input is located and to which the output files will be written.

The *Select working directory* button opens the **Select working directory** window in which the current working directory is identified as shown in [Figure 4.4](#).

The current working directory can be changed by browsing to the desired directory. Browse for instance to the <delft3d\tutorial\waq\> folder. Close the **Select working directory** window by clicking *Choose*, see [Figure 4.5](#).

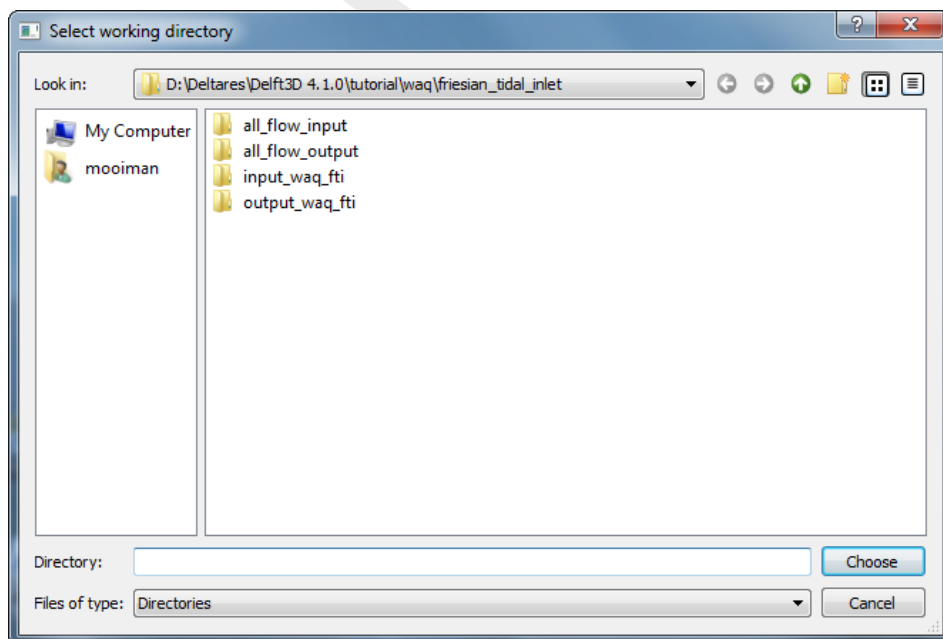


Figure 4.5: File navigation window to select a new working directory

Next the **Water quality (WAQ)** window is re-displayed, but now the changed current working directory is displayed in the title bar, see [Figure 4.6](#).

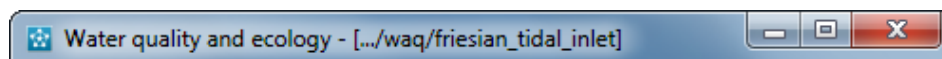


Figure 4.6: Current working directory

Creating a useful and comprehensible directory structure is worthwhile. As a water quality simulation is built up from several blocks (hydrodynamics, substances selection, discharges, etc.), a possible set-up is to store each block in a separate directory. Then it is essential that you set the working directory correctly so that the files are stored in the correct directory. A possible directory structure is shown to the right. Note that calibration runs and scenario runs are stored in separate directories.

Restriction:

- ◇ A directory name may not contain an apostrophe (').

4.4 Starting WAQ-GUI

The WAQ-GUI is started by selecting the *Define input* from the **Water quality (WAQ)** selection window. The main window of WAQ-GUI is shown in [Figure 4.8](#).

The menu bar at the top of the screen provides options for opening and saving files, for editing tables, for visualisation of the grid layout and for obtaining help.

4.4.1 Accessing data groups

A data group is accessed by clicking on the corresponding button on the left-hand side of the WAQ-GUI window. For example, clicking *Hydrodynamics* opens the data group window as shown in [Figure 4.9](#).

Clicking other datagroups in the main window will show the input screen for the respective data group. Changes made in any of the data group windows will be retained by WAQ-GUI. You will be prompted to save this data in a scenario file <*.scn> when the WAQ-GUI session is ended.

4.4.2 Saving a D-WAQ scenario file

In order to preserve changes and additions to the data groups, it is necessary to save the data defined in the data groups in a scenario data file <*.scn>. You can continue making changes and save them regularly to the scenario file. Also, the scenario file can be re-opened to edit.

If you have to define several water quality simulations in which part of the input is identical, you can simply open an existing scenario file; adapt the part that is different (e.g. different waste load) and save the scenario file under another name (preferably — but not necessarily — in another directory!). There is no need to start the input definition all over again.

You can save the scenario file by clicking menu item *File* → *Save* (or *Save As...*) in the menu bar as shown in [Figure 4.10](#). Note that the scenario file is by default saved in the

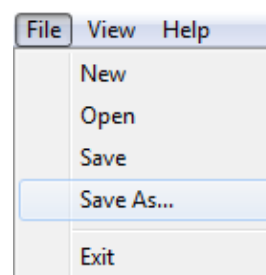


Figure 4.10: Saving the input file

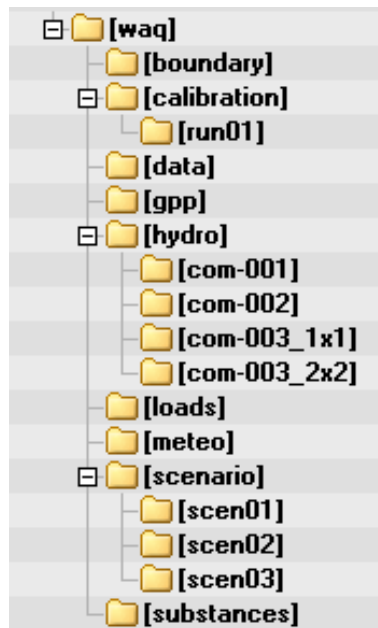


Figure 4.7: Optional directory structure for running water quality simulations

working directory you have defined earlier.

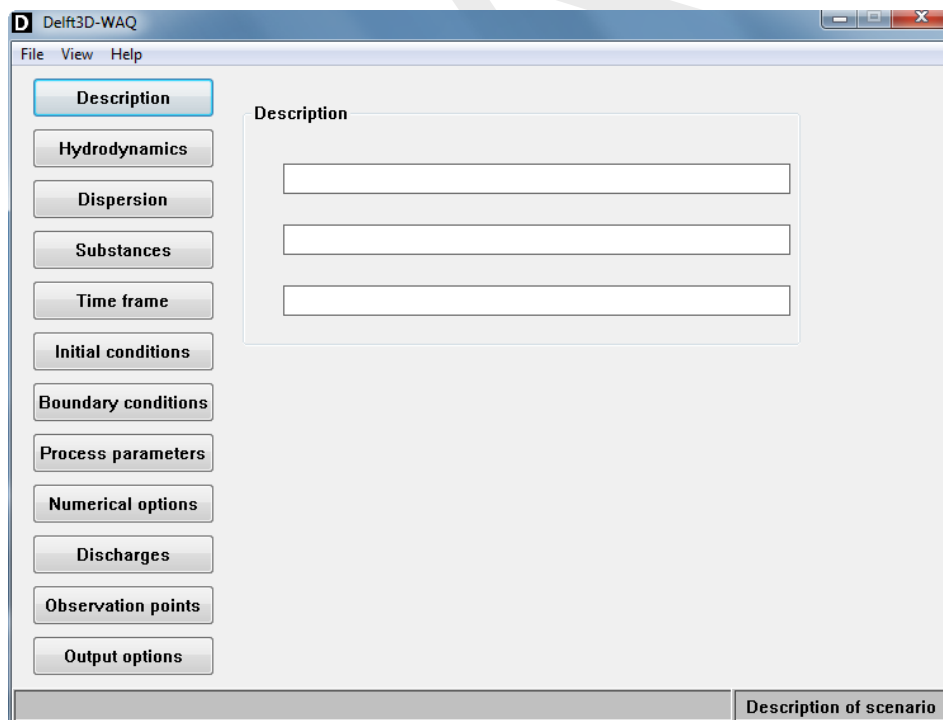


Figure 4.8: Main window of WAQ-GUI

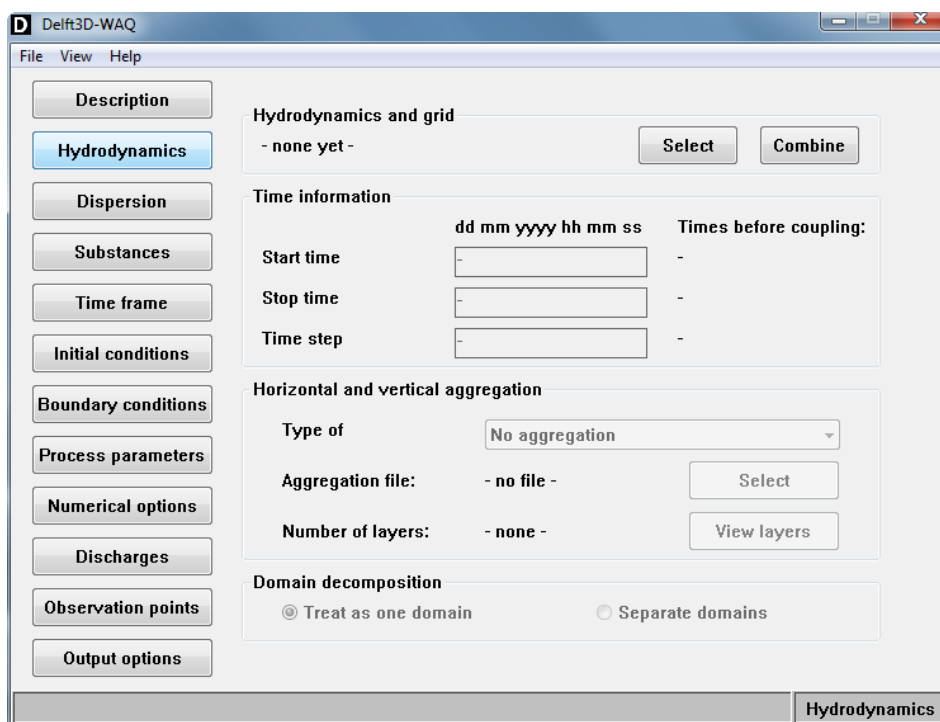


Figure 4.9: Hydrodynamics Data Group

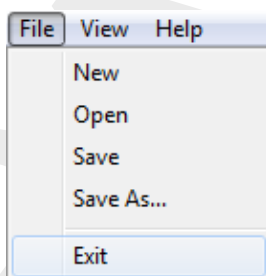


Figure 4.11: Exiting the WAQ-GUI through File → Exit

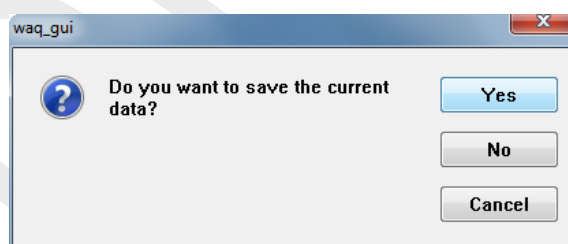


Figure 4.12: Window to save <*.scn> file before quitting

4.5 Exiting the WAQ-GUI

A WAQ-GUI session is ended by selecting *File* → *Exit* from the menu bar as shown in Figure 4.11. The GUI will first ask whether you wish to save the <*.scn> file before proceeding as shown in Figure 4.12.

After quitting WAQ-GUI, you are returned to the **Water quality (WAQ)** window. Selecting *Return* brings you back in the **Far-field water quality** selection window. Selecting *Return* again, you are back in the main **Delft3D** menu. You can then exit Delft3D entirely by selecting *Exit*.

4.6 Steps in water quality modelling

Water quality modelling with D-WAQ is very flexible. Hydrodynamics, substances, water quality processes, output variables, etc. are all free for you to choose. However, this means that you have to make decisions on what to do or what to use many times. It's best to work very structured and organised. The Delft3D-MENU and the WAQ-GUI help you with that. If you systematically go through the data groups in the order they are presented on the screen, you will automatically pass all the required input and will be 'forced' to make decisions at every point.

The basic steps in water quality modelling are:

- 1 Pick-up the result from the hydrodynamic simulation and make it suitable for application in your water quality simulation.
- 2 Define the substances and water quality processes you want to include.
- 3 Define the water quality simulation using the outcome of the first and second step. You will have to define initial conditions, boundary conditions, waste loads, simulation time, output variables, etc.
- 4 Run the simulation.
- 5 Check the output.

After step 5 you are either ready or you can return to step 1, 2 or 3 depending on the items you want to change. Usually, steps 3 to 5 are repeated multiple times.

4.7 Data flow diagram

A complete listing and description of files is given in [Appendix A](#).

Going through the steps of water quality modelling, you will pass several tools and computer programs. Output from one program can be input for another program. The tools and the files they share, are shown in [Figure 4.13](#) and [Table 4.1](#).

Table 4.1: Overview of files in D-Water Quality. Output files can be input files for other modules

| Module | Input file | Output file |
|--------------|--|---|
| Delft3D-FLOW | <*.mdf> | <com-*.dat> and <com-*.def> |
| DIDO | <*.grd> <*.dwq> | <*.dwq> |
| Couple | <com-*.dat> and <com-*.def> <*.dwq> <couplnef.inp> | <*.hyd> <com-*.flo>, <com-*.vol>, etc. <couplnef.out> |
| PLCT | <*.0> | <*.sub> <*.0> |
| WAQ-GUI | <*.hyd> <*.sub> <*.scn> <*.stt> | <*.scn> <*.inp> <*.stt> |

| Module | Input file | Output file |
|-------------------------------|--|---|
| Compute water quality | <*.inp> <com-*.flo>, <com-*.vol>, etc. | <*.lst> <*.lsp> <*.mon> <*.ada> and <*.adf> <*.hda> and <*.hdf> <*.his> <*.map> |
| Text editor (inspect results) | <couplnef.out> <*.lst> <*.lsp> <*.mon> | – |
| GPP Delft3D- QUICKPLOT | <*.ada> and <*.adf> <*.hda> and <*.hdf> <*.his> <*.map> | – |

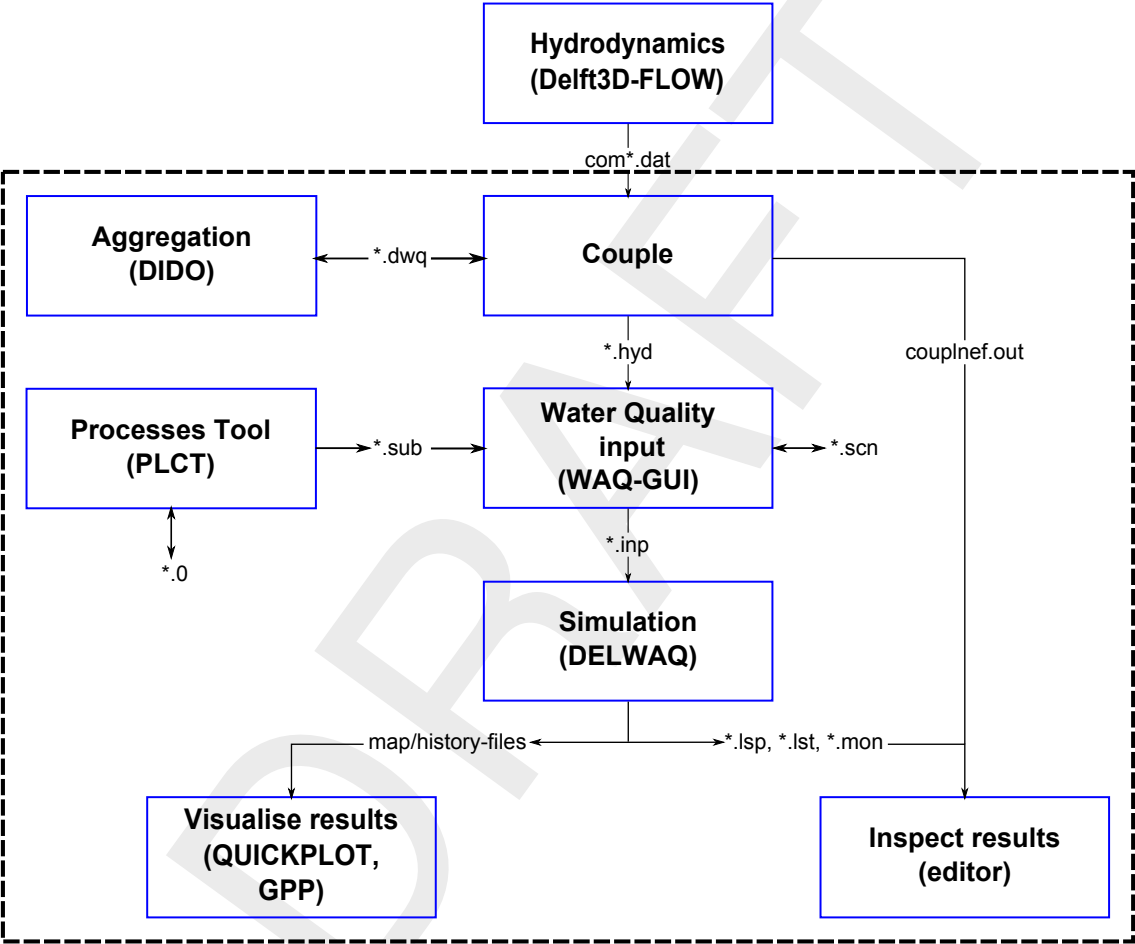


Figure 4.13: Overview of the modules and data flow diagram in D-Water Quality. Modules are shown in grey rectangles. Files they share are indicated on the arrows.

5 Graphical User Interface

5.1 Processes Library Configuration Tool (PLCT)

5.1.1 Introduction

The Processes Library Configuration Tool (PLCT) allows you to select:

- ◇ state variables (called substances in D-Water Quality)
- ◇ water quality processes
- ◇ process input parameters
- ◇ output variables

The information is stored in a PLCT file `<*.0>` which can be (re)opened in the PLCT and a substance file `<*.sub>`, which can be selected when defining a water quality simulation. It is not possible to add or remove any of these items mentioned above once you are in the WAQ-GUI (Delft3D) or WQ-module (SOBEK). For changes, you will have to return to the PLCT, make your changes, save the `<*.0>` and `<*.sub>` files and after that import the new `<*.sub>` file again in the WAQ-GUI/WQ-module.

You create a substance file in several steps:

- ◇ Choose the substance group
- ◇ Select the substances
- ◇ Select the associated processes
- ◇ Specify the input for the processes, select editable parameters and output variables
- ◇ Specify the input for the extra processes

There are many substances, processes, parameters and output variables. Basically, you have to make a choice for each and every item. Therefore, you have to work methodically through the PLCT making your choices as you go along. Remember however, that you can always return to the `<*.sub>` file and make adaptations. Also, standard substance files are available ready to use or to serve as basis for extensions ([Appendix B](#)).

To work with the PLCT and the water quality processes it is essential that you are familiar with the mathematical formulation of the processes. When you see a process for the first time, refer to the accompanying description in the Technical Reference Manual ([D-WAQ TRM, 2013](#)) for an explanation of parameters and for directives for use.

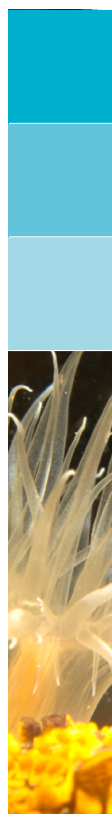
5.1.2 Opening the PLCT

Opening the PLCT (SOBEK)

You can set or change the configuration of the Processes Library with the help of the Processes Library Configuration Tool (PLCT).

- ◇ Tick "Do not use predefined processes" and click the "Define Processes:" *Edit* button in the "Processes" tab form.

The PLCT is started.



Opening the PLCT (Delft3D)

Clicking *Processes* in the **Water quality and ecology** window and then the *ECO* button, the PLCT will open in ecology mode (ECO, use BLOOM algae).

5.1.3 Processes Library Configuration Tool (PLCT)

Initially, the PLCT consists of three windows (Figure 5.1):

- 1 **Processes Library Configuration Tool** File managing window for opening and saving files and exiting the PLCT. The window also gives an overview of the substances selected so far.
- 2 **Select Groups** Overview of available substances groups, and entry point to select substances. Also, entry point to Extra processes
- 3 **Messages** Window displays messages when errors occur, mostly related to missing information.

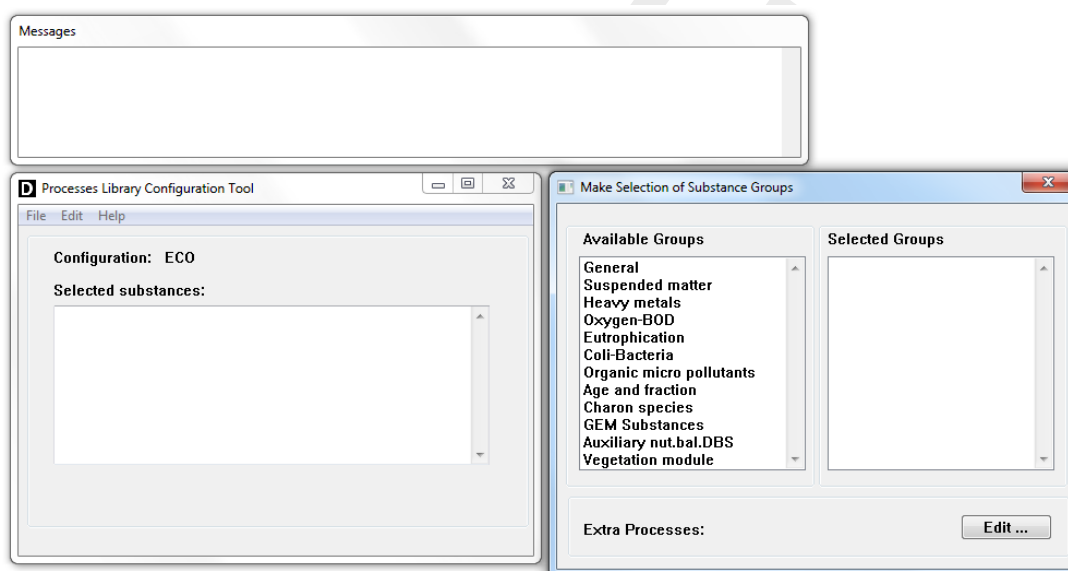


Figure 5.1: Main windows of the Processes Library Configuration Tool

The **Processes Library Configuration Tool** window displays the version number, the name of the file you are currently working on and the configuration (ECO, WAQ). Note that a `<*.0>` and `<*.sub>` file generated for example with the ECO configuration, can not be opened automatically in the WAQ configuration. The configuration is included in the first line of the `<*.0>` file (for example configuration 'ECO') and can be changed manually here (e.g. configuration 'WAQ'). The PLCT will give a warning when you try to open the `<*.0>` file.

The menu bar has the following options:

| | | |
|-------------|----------------|---|
| <i>File</i> | <i>New</i> | Start a new scenario — clear all input. |
| | <i>Open...</i> | Open an existing PLCT <code><*.0></code> file. |
| | <i>Save</i> | Save the current PLCT <code><*.0></code> file using the previously given name, or the default name <code><substate.0></code> . A substance file <code><*.sub></code> is saved simultaneously. |

Save as... Save the current PLCT <*.0> file and specify its filename. A substance file <*.sub> is saved simultaneously.

Exit Exit the PLCT.

Select groups

The **Make Selection of Substances Groups** window has three parts:

- 1 **Available Groups** Shows the available substance groups within the configuration selected.
You can select a specific group by a mouse click or standard keyboard controls. Selected substance groups will be displayed in the **Selected Groups** part on the right side of the window. Multiple groups can be selected by holding the Control key on your keyboard and selecting the second or further substance group.
- 2 **Selected Groups** Substance groups that are highlighted in the **Available Groups** on the left side of the window are displayed. Clicking on one of the selected substance groups here opens the **Make Selection of Substances** window, displaying the substances that are included in the substance group.
- 3 **Extra Processes** Clicking *Edit...* opens a window with all the Extra processes that are required for the water quality processes.
Extra Processes are processes that do not calculate a mass flux on one of the selected substances. This can be for post-processing purposes (e.g. calculating Total-Nitrogen), but lump mass fluxes as well (e.g. total resuspension).

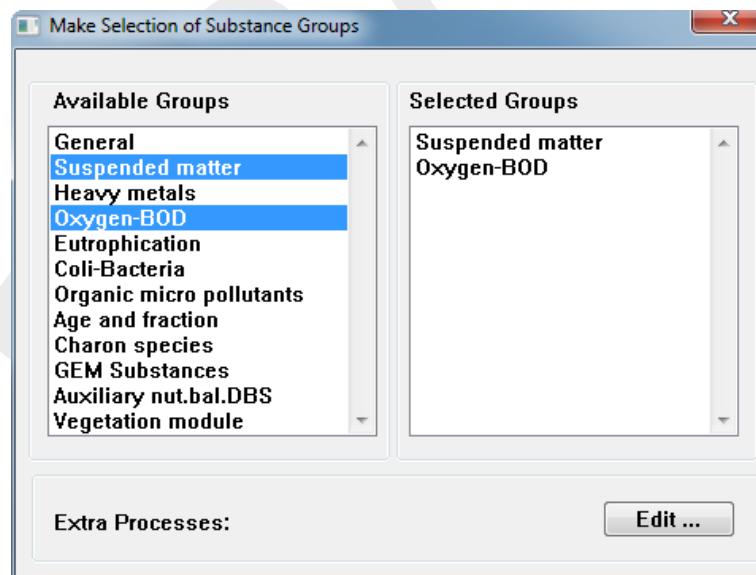


Figure 5.2: Select Groups window of the PLCT. Highlighted groups 'Suspended matter' and 'Oxygen-BOD' are selected and displayed in the right side column

Select substances

The **Make Selection of Substances** window works analogous to the **Make Selection of Substances Groups** window. Every substance group has its own **Select Substances** window. If you have selected multiple substance groups, you have to select the substances per group separately.

You can select available substances by a mouse click or standard keyboard controls. Selected substances will be displayed in the *Selected substances* part on the right side of the window. Multiple substances can be selected by holding the **CTRL**-key on your keyboard and selecting the second or more substance by mouse.

Clicking on one of the available substances opens the **Select Processes** window, displaying all the water quality processes that are available for this substance.

Clicking *Ready* closes the window and bring you back to the **Select Substance Group** window.

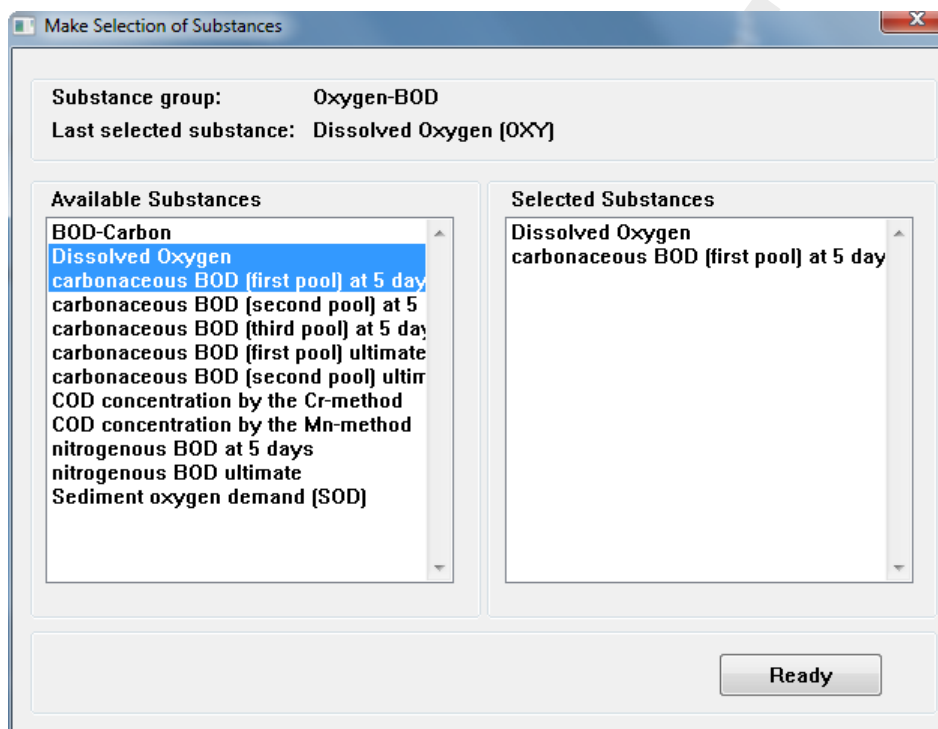


Figure 5.3: Select Substances window for the Oxygen-BOD group. Highlighted substances 'Dissolved Oxygen' and 'Carbonaceous BOD (first pool) at 5 days' are selected and displayed in the right side column

Select processes

The **Select Processes** window displays all processes that are available for the selected substance (Figure 5.4). You can select or 'activate' a process by checking the check box behind the process. An *Edit...* button will appear. Checking the check box once again, deactivates the process and *Edit...* will disappear. By clicking *Edit...*, you will open the **Specify Process** window (see Figure 5.5, also next section).

Occasionally, instead of the *Edit...* button, a *Define...* button will appear. A *Define...* button is displayed when the input for that specific process is not completely defined and your input is required: the **Specify Process** window will open automatically in this case. An *Edit...* button indicates that there is no missing input. There is no check on the correctness on the input, only on the completeness of the input.

After selecting and editing all required processes, you can close the **Select Processes** window by clicking *Ok*. Clicking *Cancel* will loose all changes you made since opening the window. No warning is given.

If the number of available processes is more than 12, the *Scroll Up* and *Scroll Down* buttons enable you to go through the listing of the processes.

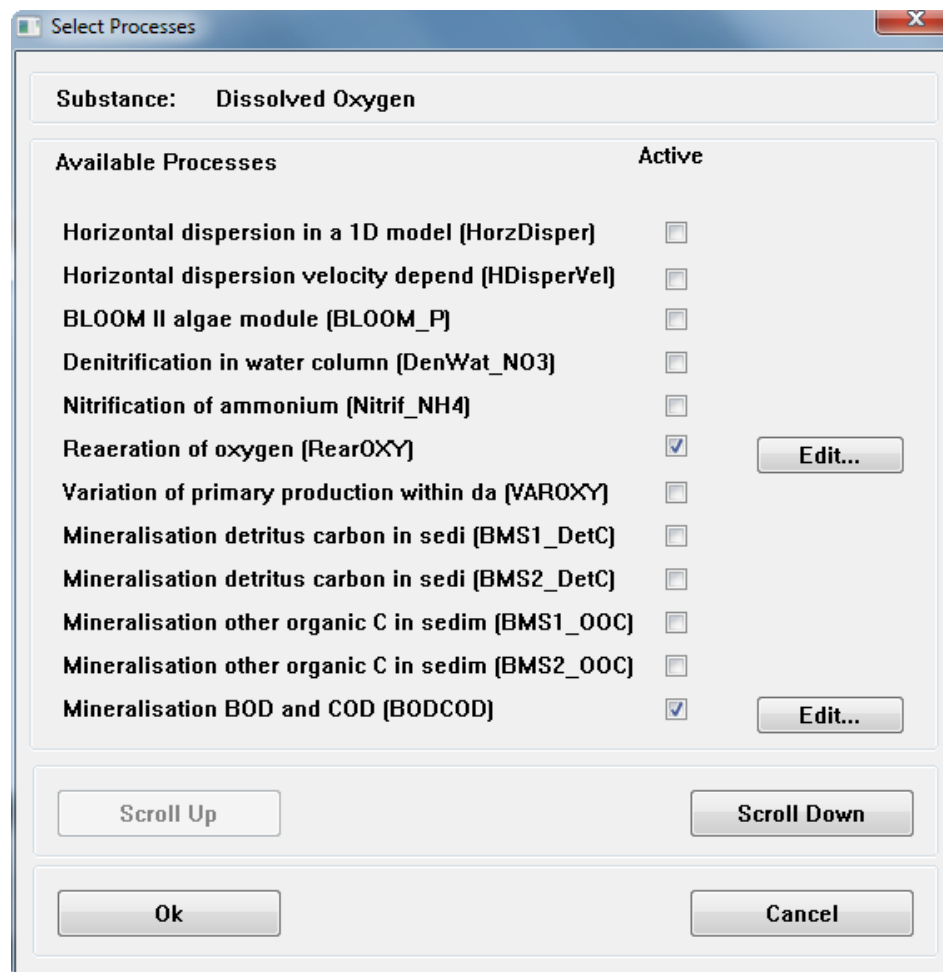


Figure 5.4: Select Processes window for 'Dissolved Oxygen'. Activated process are checked and an Edit... button is shown

Specify process

The **Specify Process** window is opened by clicking *Edit...* in the **Select Processes** window. The information on the **Specify Process** window is divided in six columns:

- 1 Description and name of the process parameter
- 2 Type of process parameter

Two options:

- ◇ Constant
- ◇ Derived from another process

A list box indicates that you have the option to make the process parameter a constant or to derive it from another process. If no list box is available, the process parameter can not be derived from another process and automatically is a constant.

- 3 Value of the process parameter

- ◇ When the process parameters is defined as a constant, the default value is shown. '-999' is identified as a missing value, and you will have to define a value.
- ◇ *Modelled*: the process parameter is chosen as a substance or the process parameter is available from the hydrodynamic simulation (e.g. Volume).

| Process: Reaeration of oxygen (RearOXY) | | | Unit | Editable | Output |
|---|----------|------------|--------|--------------------------|--------------------------|
| Input / Output parameters | | | | | |
| Salinity (Salinity) | Constant | 35 | [g/kg] | <input type="checkbox"/> | <input type="checkbox"/> |
| Dissolved Oxygen (OXY) | | Modelled | [g/m3] | | |
| depth of segment (Depth) | DynDepth | (DynDepth) | [m] | | <input type="checkbox"/> |
| ambient water temperature (Temp) | Constant | 15 | [oC] | <input type="checkbox"/> | <input type="checkbox"/> |
| horizontal flow velocity (Velocity) | Veloc | (Veloc) | [m/s] | | <input type="checkbox"/> |
| wind speed (VWind) | Constant | 3 | [m/s] | <input type="checkbox"/> | <input type="checkbox"/> |
| switch for oxygen reaeration formulation (SWRear) | Constant | 1 | (-) | <input type="checkbox"/> | <input type="checkbox"/> |
| reaeration transfer coefficient (KLRear) | Constant | 1 | [m/d] | <input type="checkbox"/> | <input type="checkbox"/> |
| temperature coefficient for reaeration (TCRear) | Constant | 1.016 | (-) | <input type="checkbox"/> | <input type="checkbox"/> |
| timestep for processes (DELTA) | | Modelled | [d] | | |

Scroll Up Scroll Down

Ok Cancel

Figure 5.5: Specify Process window for the Reaeration of oxygen

- ◇ Output: the process parameter is an output variable only, and no input value is required.
 - ◇ (Text string between brackets): the process parameter is derived from another process. The process name is indicated between brackets.
- 4 Unit
Unit of the process parameter
 - 5 Editable check box
Only available for process parameters defined as Constant. Checking the Editable box will save the process parameter to the <*.0> and <*.sub> files. In the WAQ-GUI under *Process Parameters*, these process parameters can be given a constant value other than the default value, a time-series or a segment function. For process parameters that are not made editable the default value will be used in the water quality simulation.
 - 6 Output check box
Checking the Output box will save the process parameter to the <*.0> and <*.sub> files as output variables. The value of the process parameter will be written to the respective output files during a water quality simulation.

After selecting and editing all required process parameters, you can close the **Specify process** window by clicking *Ok*. Clicking *Cancel* will loose all changes you made since opening the window. No warning is given.

If the number of available process parameters is more than 12, the *Scroll Up* and *Scroll Down* buttons enable you to go through the listing of the process parameters.

Each process has its own description and directives for use, see Technical Reference Manual (D-WAQ TRM, 2013).

Extra processes

Finally, after you have selected all the substance groups, the substances, their processes and the process parameters, you have to check the *Extra Processes*. The PLCT automatically accumulates all processes that do not directly calculate mass fluxes of substances. These processes are compiled in the **Specify Extra Processes** window. The window is analogous to the **Select Processes** window, with the exception that you are not allowed to deactivate processes here. If you want to deactivate an extra process, you have to go to the location in a **Specify Process** window where the process is selected. The process parameter should be changed to constant, instead of being derived from the (extra) process.

Clicking *Edit...* opens a **Specify Process** window.

Note that new extra processes can be added as well if you make such a change in a **Specify Process** window. You should check the Extra Processes list for new extra processes.

When finished you can save the PLCT file <*.0> and simultaneously a substance <*.sub> file will be saved. Exit the PLCT through *File* → *Exit*.

Substances and processes not supported by the WAQ-GUI

Substances and processes not supported by the WAQ-GUI but present in the Processes Library can be added by manual editing. Two additional user manuals are available for this: [D-WAQ TRM \(2013\)](#) and [D-WAQ Input file \(2013\)](#).

5.2 Using the hydrodynamic result (Delft3D)

The transport of substances is based on a Delft3D-FLOW ([Delft3D-FLOW UM, 2013](#)) or D-Flow FM ([D-Flow FM UM, 2015](#)) result, though coupling to other three-dimensional hydrodynamic models, such as UNTRIM and TELEMAC is possible as well. Delft3D-FLOW generates either a so-called communication file, consisting of a data file and a definition file and containing the "raw" hydrodynamic information that needs to be converted by an auxiliary program (the coupling program) or, via a builtin coupling procedure, a set of ready-to-use files.

Method 1: the builtin coupling

The *builtin coupling* is the preferred mode of coupling Delft3D-FLOW to D-Water Quality. With this mode the required input files with the grid layout and the hydrodynamic results are written directly and therefore a separate coupling step is not needed anymore. There is one drawback: you have to decide at the start of the hydrodynamic calculation how to aggregate in time and space (both horizontally and vertically). The other method allows you to store the full result of the hydrodynamic calculation in so-called communication files and do the coupling afterwards.

This method can also be used for 'classic' domain decomposition Delft3D-FLOW calculations with multiple grids, and for automatic parallel calculations of Delft3D-FLOW.

The builtin coupling is enabled in Delft3D-FLOW via the user-interface using the *Export WAQ input* checkbox and the *Edit WAQ input* button.

This method can also be used for 'classic' domain decomposition Delft3D-FLOW calculations with multiple grids, but doesn't work for automatic parallel calculations of Delft3D-FLOW. The output should encompass a representative period with a sufficient time resolution. Examples of a representative period are a single tide and a spring-neap cycle. A time resolution is suf-

ficient when the essence of the hydrodynamic system is described. For example, a repeating 12 hours tidal cycle should have a maximum time resolution of one hour. A larger time step would filter out some of the tidal essence of the system.

Method 2: the communication file

The so-called communication file actually consists of two files. The filenames are always <com-*.dat> and <com-*.def> respectively, where '*' indicates a run ID of the Delft3D-FLOW simulation.

D-WAQ allows you to extend the simulation beyond the period stored in the communication file. When it reaches the end of the period, D-WAQ will rewind the hydrodynamic file and repeat it (Figure 5.6) until it reaches the end of the D-WAQ simulation.

As D-WAQ will rewind the hydrodynamic result, it is important that the start and the end of the representative period are similar. In Figure 5.6(A) the water level is the same at the start and the end. If only 6 hours were stored on the communication file, rewinding would result in a water level as shown in Figure 5.6(B). Obviously, this is incorrect, but D-WAQ does not check this *closure error*. You should check this yourself by plotting the change in water level due to a rewind.

Hydrodynamic modelling usually requires a more detailed schematisation or grid than water quality modelling. Therefore, generally it is allowed to reduce the number of computational cells in the water quality modelling. This process is called aggregation. Aggregation is divided in horizontal aggregation and vertical aggregation (Figure 5.7).

Aggregation of the hydrodynamic results inevitably results in loss of information. This is not necessarily a problem. It is up to you to decide if the aggregation is allowed. For example, if stratification is essential in your water system you should not use vertical aggregation to obtain a 2DH schematisation. A good check on aggregation is to repeat the salinity simulation that was carried out with Delft3D-FLOW, with D-Water Quality. When you use exactly the same input (initial condition, boundary conditions, etc.) the results should be the same or very similar. If the deviation is too large, one reason could be that the aggregation has led to too coarse a grid. Other reasons can be numerical problems, or too large a time step.

5.2.1 Couple GUI

To couple a hydrodynamic result select *Coupling* from the **Water quality (WAQ)** window (Figure 4.3). From the **Hydrodynamic coupling** selection window first select *Define input*, see Figure 5.8. When you need a coupling from a domain decomposition hydrodynamic simulation you have to define the input for each domain separately.

Next, the window in Figure 5.9 appears, the COUP-GUI. As you will see later, the window is exactly the same as the Delft3D-WAQ GUI, with the difference that many option are not sensitive. Only three data groups are sensitive: *Description*, *Hydrodynamics* and *Dispersion*.

The menu bar has three options:

| | | |
|-------------|--------------------|---|
| <i>File</i> | <i>New</i> | Start a new scenario — clear input in all data groups |
| | <i>Open</i> | Open an existing scenario <*.hyd> file |
| | <i>Save</i> | Save the current scenario file using the previously given name, or the default name <com-*.hyd> |
| | <i>Save As ...</i> | Save the current scenario file and specify its filename |
| | <i>Exit</i> | Exit the GUI |

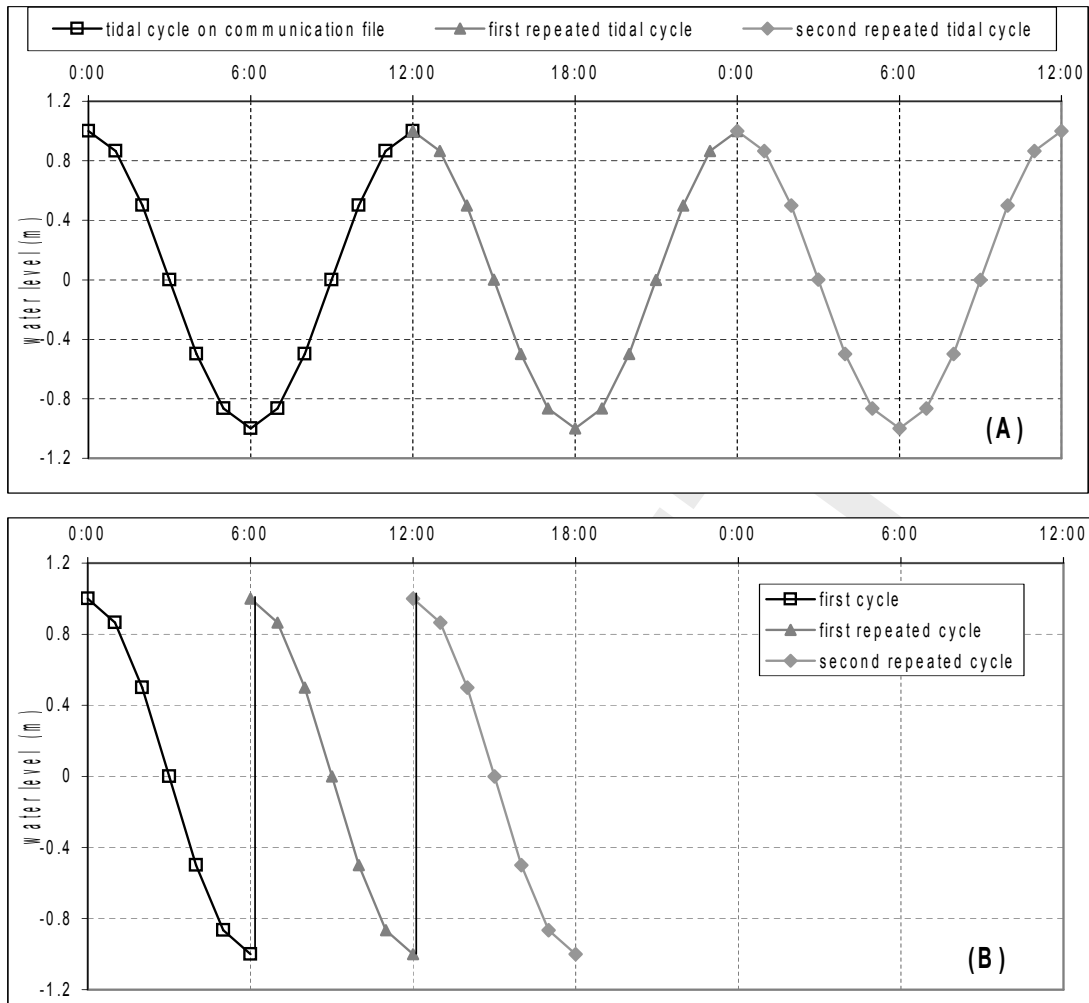


Figure 5.6: (A) Correct repetition of a tidal cycle of 12 hours stored on the communication file, for a D-WAQ simulation of 36 hours. (B) Incorrect repetition of a hydrodynamic cycle; rewinding results in a major jump in water level.

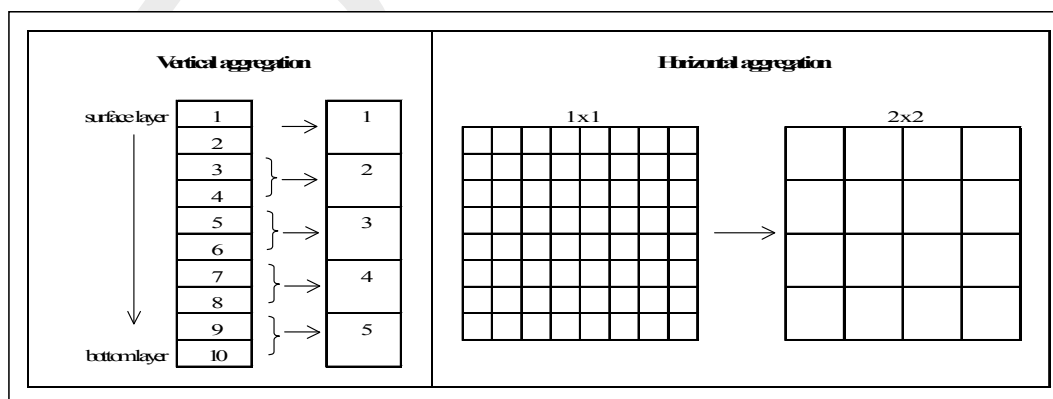


Figure 5.7: Principle of vertical and horizontal aggregation. Here the vertical aggregation combines 10 layers in the hydrodynamic simulation to 5 layers in the water quality simulation. The horizontal aggregation combines 4 computational cells in the hydrodynamic simulation to 1 computational cell in the water quality simulation.

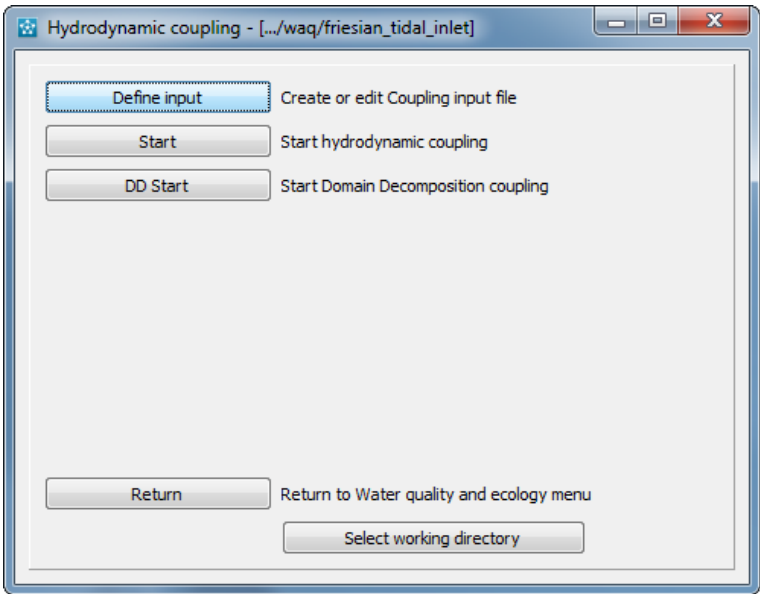


Figure 5.8: Hydrodynamic coupling selection window

| | | |
|------|---------------------------|--|
| View | Disabled in coupling mode | |
| Help | Contents | Opens the general help menu of D-Water Quality |
| | About | Displays the version number of the GUI |

5.2.2 Description

Selecting *Description* opens a screen in which you can enter three lines of text. The lines can be used to describe the coupling/aggregation. The maximum length of each of the lines is 39 characters.

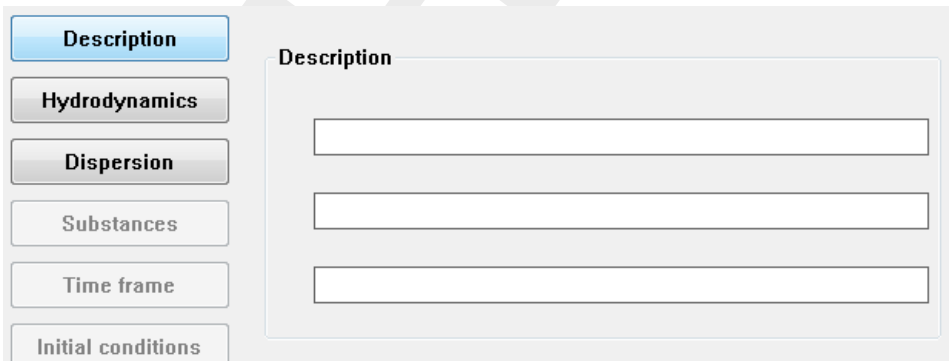


Figure 5.10: Description window with three lines. The maximum length of the description lines is 39 characters

5.2.3 Hydrodynamics

The **Hydrodynamics** window has four frames:

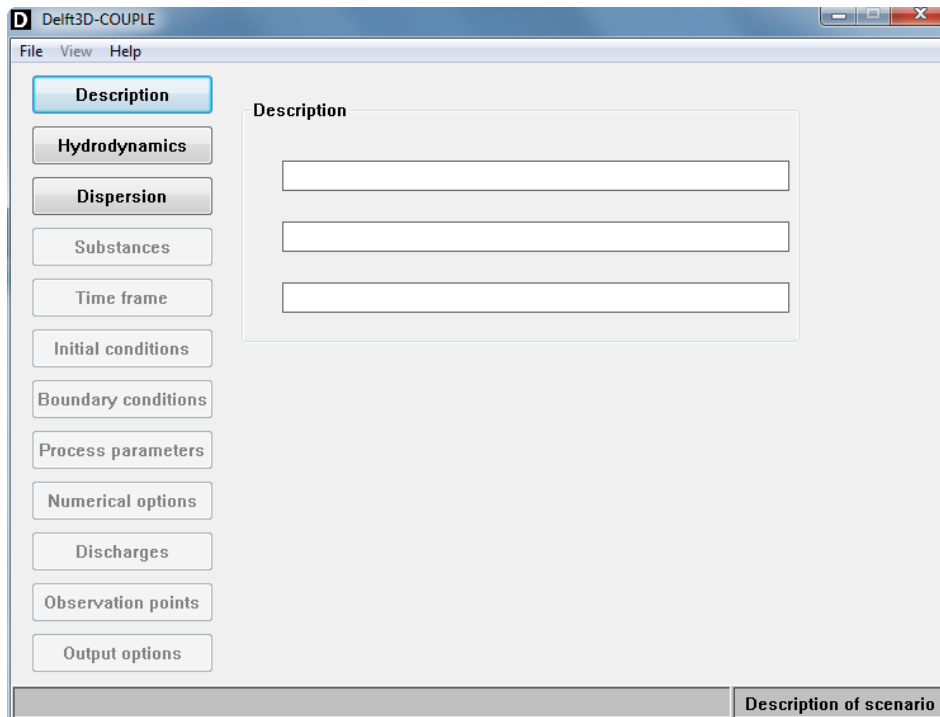


Figure 5.9: Opening screen of the COUP-GUI

- 1 **Hydrodynamics and grid** Select the hydrodynamic communication file <com-*.dat> or the domain decomposition file <*.ddb>. This automatically results in setting the grid schematisation. Clicking *Com-file* opens a file browser, which enables you to select a <com-*.dat> file. Note that it is not required that the <com-*.dat> file is located in the working directory. Clicking *DD-bound* opens a file browser, which enables you to select a <*.ddb> file.
- 2 **Time information** After selecting the communication file, this part shows the times stored in the communication file (start time, stop time and time step). Also, three input fields allow you to set the start time, stop time and time step for the coupling.
- 3 **Horizontal and vertical aggregation** You have to select the horizontal aggregation here. Choices are explained below. Furthermore, set the vertical aggregation (combining hydrodynamic layers).
- 4 **Domain decomposition** The multiple FLOW domains can be combined to 1 (one) water quality domain, or, treated as separate domains.

Hydrodynamics and grid

...\\com-tut_fti_waq.dat Com-file DD-bound

Time information

| | dd mm yyyy hh mm ss | Times before coupling: |
|------------|---------------------|------------------------|
| Start time | 05 08 1990 12 30 00 | 05 08 1990 12 30 00 |
| Stop time | 06 08 1990 01 00 00 | 06 08 1990 01 00 00 |
| Time step | 00 00 0000 00 15 00 | 00 00 0000 00 15 00 |

Horizontal and vertical aggregation

Deltares **Type of** No aggregation 63 of 378

Aggregation file: - no file - Select

button, give the name of the ddb-file that was produced during the run, and answer 'yes' to the question: 'Has this ddb-file been created by a MPI-based parallel Delft3D FLOW run (y/n)?'.

Instead of individual communication files (such as <com-f35_waq.dat>) you now select a file describing the relation between the various domains. The names of the communication files that belong to each domain are derived from this information.

Once you have selected this "DD-bound" file, the user-interface is capable of dealing with all domains at once. In fact, as far as possible the user-interface tries to hide the distinction between single-domain and multi-domain databases. This is not always possible due to the nature of the conversion process.

Time information

The right side of the frame displays the times stored in the hydrodynamic communication file. The start time, stop time and time step to be stored in the coupled hydrodynamics can be specified.

The *Start time*, *Stop time* and *Time step* of the coupled hydrodynamics have to satisfy the following conditions:

- ◇ The start time of the coupled hydrodynamics has to be equal to or later than the start time in the communication file.
- ◇ The start time of the coupled hydrodynamics has to be before the stop time in the communication file.
- ◇ The stop time of the coupled hydrodynamics has to be before or equal to the stop time in the communication file.
- ◇ The stop time of the coupled hydrodynamics has to be later than the start time in the communication file.
- ◇ The stop time in the coupled hydrodynamics has to be later than the start time in the coupled hydrodynamics.
- ◇ The time step in the coupled hydrodynamics has to be equal to or an integer multiplication of the time step in the communication file. So if the time step in the communication file is 15 minutes, the time steps allowed in the coupled hydrodynamics are 15 minutes, 30 minutes, 45 minutes, 1 hour, etc.
- ◇ The total time between the start time and the stop time in the coupled hydrodynamics has to be an integer multiplication of the time step in the coupled hydrodynamics.

Finally, if the hydrodynamic simulation contains walking discharges, aggregation of the time step is not allowed. A warning is given when you try to couple anyway.

Horizontal and vertical aggregation

There are three options for the horizontal aggregation of the hydrodynamic grid:

- | | |
|--|--|
| 1 No aggregation (e.g. for D-Waq PART) | No aggregation is applied, the hydrodynamic grid will be coupled horizontally unchanged. This option is required if you want to use numerical schemes 4, 19 or 20 (refer to section 10.5), or if you want to run D-Waq PART. (D-Waq PART makes use of the same Coupling procedure). |
| 2 Use aggregation file (DIDO) | If you select this option the <i>Select</i> button will be activated. Clicking <i>Select</i> opens a file browser, in which you have to select the DIDO <*.dwq> aggregation file you have prepared with DIDO. |

- | | |
|-------------------------|--|
| 3 Remove inactive cells | No horizontal aggregation is applied and as such this option is equal to the first option. Inactive computational cells such as dry points or cells lying on the land are excluded. The benefits of this option are the reduced file sizes of the coupled hydrodynamics and some D-WAQ output files. However, you can not use numerical schemes 19 or 20 with this option. |
|-------------------------|--|

The aggregation tool DIDO can be started from the *Tools* menu. Please refer to the DIDO manual ([DIDO UM, 2013](#)) on how to prepare a `<*.dwq>` file. Note that it is not required that the `<*.dwq>` file is located in the working directory.

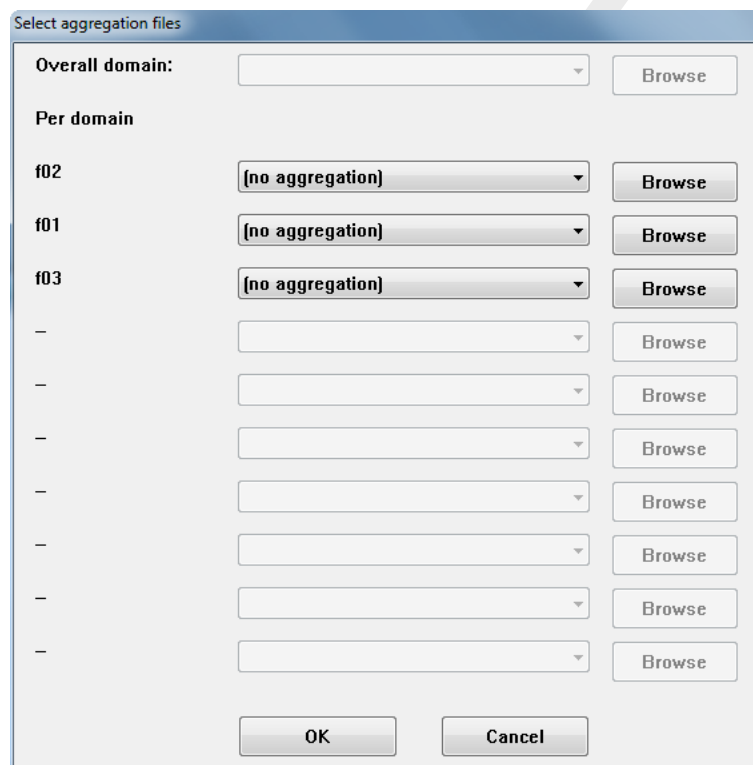


Figure 5.12: *Select aggregation files* window in case of DD models

If you select a multi-domain hydrodynamic database, then aggregation will be done per domain, see [Figure 5.12](#):

- ◇ You select an aggregation file created by DIDO for a particular domain;
- ◇ or you decide not to use an aggregation file. To keep the aggregation options for all domains consistent, the option *Remove inactive cells* is turned on instead.

To vertically aggregate layers click *Edit layers*. The **Layer editor** window will open listing the number of layers in the hydrodynamic simulation. When you open the screen for the first time, by default each layer in the coupled hydrodynamics is set equal to one layer in the hydrodynamic simulation. Note that a 2DH hydrodynamic simulation has no possibility for vertical aggregation.

[Figure 5.13](#) shows the **Layer editor** for a hydrodynamic simulation that has 5 layers. By entering an integer number in one of the input boxes, you indicate the number of hydrodynamic layers that have to be included in the specific water quality layer. In [Figure 5.13](#) the first layer in the water quality simulation contains the first and second hydrodynamic layers. The second

layer in the water quality simulation contains the third and fourth hydrodynamic layers. The third layer in the water quality simulation contains the fifth hydrodynamic layer. Entering a number greater than 1, means that water quality layers will be removed from the bottom (note that layer 1 is the surface layer). Lowering the number in a text box, means that water quality layers will be added at the bottom. The sum of the hydrodynamic layers will always be equal to the original number of layers, e.g. $(10 * 1) = (3 + 2 + 2 + 2 + 1)$ in Figure 5.13.

| Water quality layer | Hydrodynamic layers |
|---------------------|---------------------|
| 1 | 1 |
| 2 | 1 |
| 3 | 1 |
| 4 | 1 |
| 5 | 1 |
| 6 | 1 |
| 7 | 1 |
| 8 | 1 |
| 9 | 1 |
| 10 | 1 |

| Water quality layer | Hydrodynamic layers |
|---------------------|---------------------|
| 1 | 2 |
| 2 | 2 |
| 3 | 2 |
| 4 | 2 |
| 5 | 2 |

Figure 5.13: Layer editor. Left screen shows the original 10 hydrodynamic layers. The right screen shows a vertical aggregation into 5 layers that will be applied in the water quality simulation.

You are not allowed to enter a zero; a warning will be given if you do. Also, if the number you enter is higher than the number of hydrodynamic layers available, a warning will be given and the number will be truncated to the maximum allowed.

When coupling to a multi-domain hydrodynamic database, certain restrictions hold. This can be best described via an example. Suppose you have three domains:

- ◇ One with three layers (40, 40 and 20 % of the total depth)
- ◇ One with six layers (20, 20, 20, 20, 10 and 10 % of the total depth)
- ◇ One with two layers (40 and 60 % respectively)

| Domain 1 | Domain 2 | Domain 3 |
|----------|----------|----------|
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |

Only those interfaces that run through all domains without a jump can be maintained in the final conversion. So in the above situation, the three domains will result in a *two-layers* system, defined by the third domain.¹

Domain decomposition

You have two options for the actual conversion²:

- ◇ Merge the domains into a single one, so that the subsequent water quality computation works on a single domain. Numerical schemes 19 and 20 are not allowed in this case.
- ◇ Convert the hydrodynamic databases separately per domain. In that case the water quality computation will be done in a multi-domain mode too.

Warning:

- ◇ The second option is not implemented yet.
Even in the first case it will still be possible to run the water quality module on individual domains (in that case you simply select the hydrodynamic description for that particular domain and there is no relationship with the others).



5.2.4 Dispersion

The following only applies for a 3D hydrodynamic database.

Clicking *Dispersion* opens the window shown in [Figure 5.14](#). Note that, any value that you enter here, can still be changed when you define the input for a water quality simulation.

The coupling automatically takes over the vertical dispersions calculated by the hydrodynamic model. However, as these values may be unrealistically small, you can enter a minimal value for the vertical dispersion here. The text boxes become active when you check the *Use minimum values* box. The water column can be split. You can enter a different value below and above a certain interface, including the depth of this interface.

5.2.5 Running the coupling

Once you have defined the conversion of the hydrodynamic `<com-*.dat>` file, you can save the coupled hydrodynamics file `<*.hyd>` by selecting *File* → *Save* or *File* → *Save As...*. Default the name of the coupled hydrodynamics file is `<com-*.hyd>`. *We advise you to save the `<*.hyd>` file in the **working directory**.*

Leave the COUP-GUI by selecting *File* → *Exit* in the menu bar. When you need a coupling from a domain decomposition hydrodynamic simulation you have to define the input for each domain separately.

Back in the **Hydrodynamic coupling** selection window (see [Figure 5.8](#)), select *Start* or *DD Start* to execute the coupling. Information about the coupling will be displayed in a new window. You can close this window when the coupling has finished.

Information on the coupling is written to the `<couplnef.out>` or `<name-ddcouple.out>` file. You can check this file. First select *Return* in the **Hydrodynamic coupling** selection window; you will be back in the **Water quality (WAQ)** selection window. From this window select the

¹(april 2005) It is possible to create sets of layer thicknesses that would result in a single layer. Unfortunately the user-interface will currently report an error, rather than revert to a single layer.

²(april 2005) The multi-domain option is not fully supported yet. Use the single-domain for the moment.

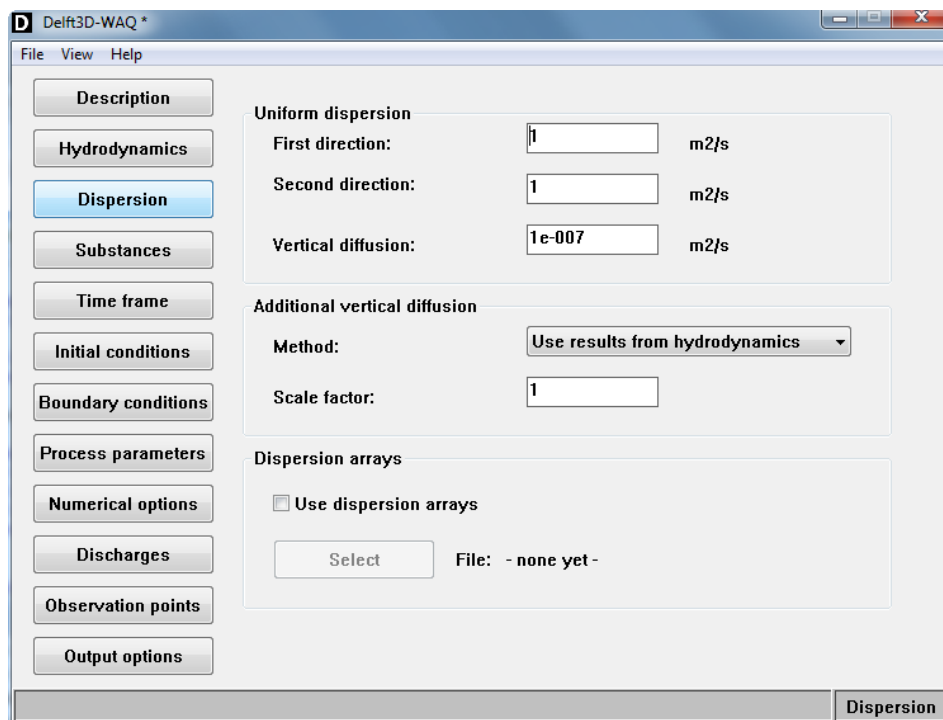


Figure 5.14: Dispersion window in the COUP-GUI

Reports item. The **View report files** selection window will then open, see Figure 5.15.

From the **View report files** window select *Coupling* to view the information on the coupling.



Remark:

- ◇ The coupled hydrodynamics and the file <couplnef.out> or <name-ddcouple.out> is stored in the working directory.

Important information you get from the coupling, is the minimum residence time. Explicit numerical schemes require that the time step in the water quality simulation is smaller than the minimal residence time (also refer to Chapter 10). The excerpt of the <couplnef.out> file displayed below indicates that the minimal residence is 498.1 seconds.

5.3 Define input (Delft3D): WAQ-GUI

Select *Define input* (Figure 4.3) to start the input procedure for the water quality calculation. The main window is visualised in (Figure 5.16).

The Graphical User Interface for water quality calculations consists of:

- ◇ The menu items: *File*, *View*, *Tools* and *Help*
- ◇ The data groups: *Description*, *Hydrodynamics*, *Dispersion*, *Substances*, *Time frame*, *Initial conditions*, *Boundary conditions*, *Process parameters*, *Numerical options*, *Discharges*, *Observation points* and *Output options*
- ◇ Additional information in the bottom row of the window, like version number and identification of data group you are working in

To prepare a water quality calculation all data groups must be specified. It is recommended to follow the order in which they appear (from top to bottom) in the main window, although this is

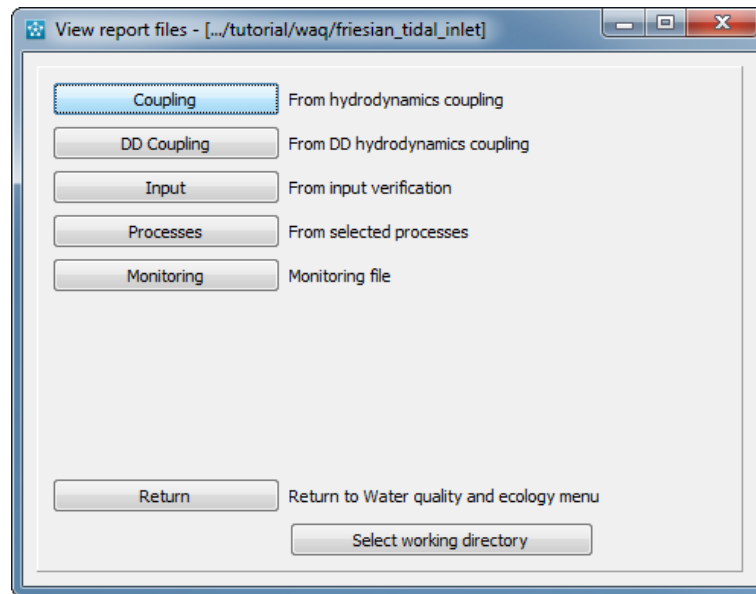


Figure 5.15: View report files selection window

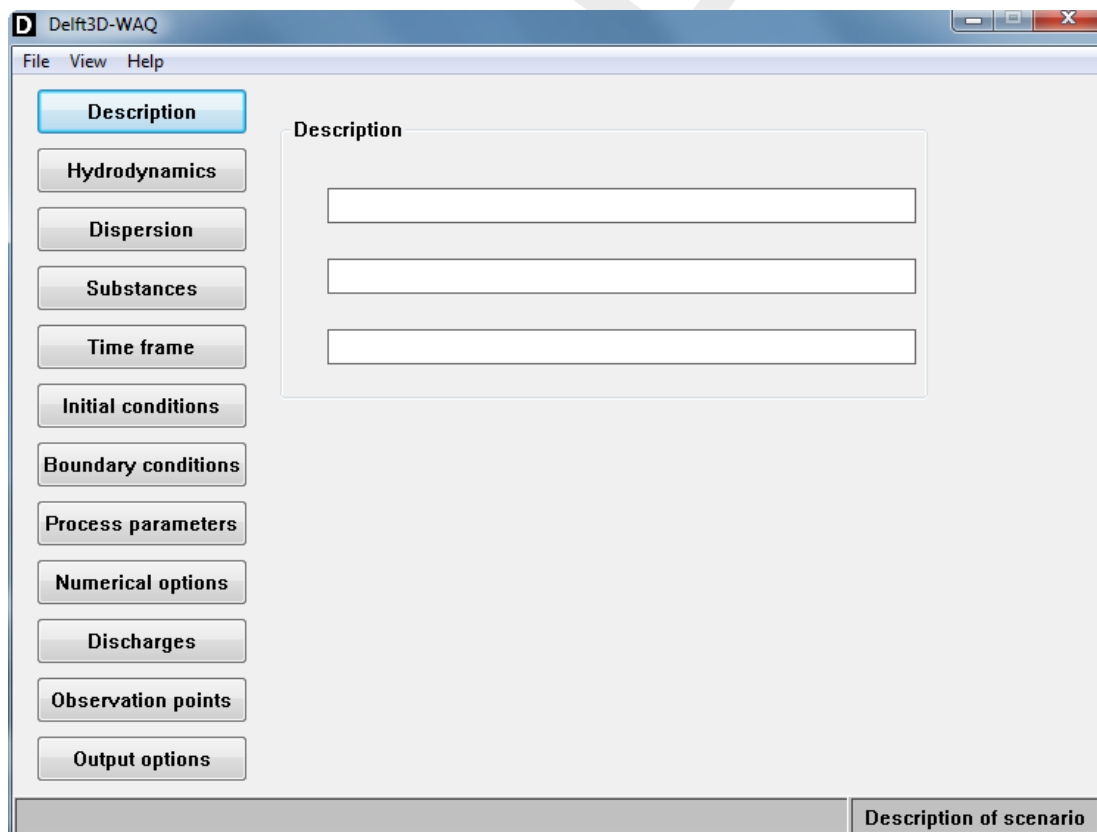


Figure 5.16: Main window of the WAQ-GUI. The buttons on the left side of the window represent distinct data groups.

not obliged. After selecting one of the data groups, the right side of the window will show the data specification for that data group. When you select another data group information will be saved automatically.

The menu bar has four options:

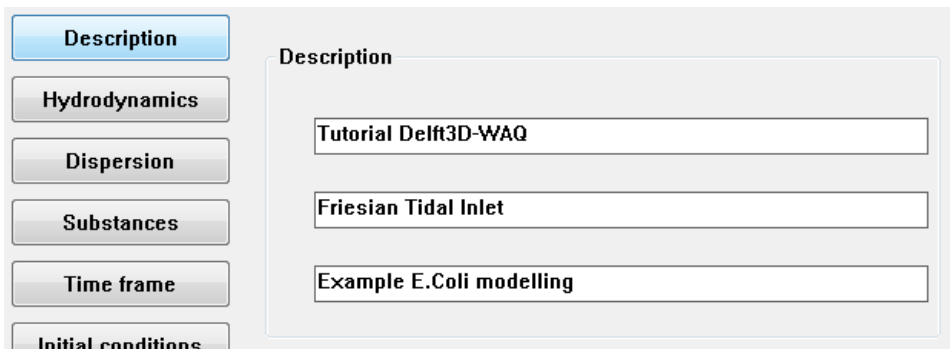


Figure 5.17: Description Data Group. The maximum length of the text is 39 characters

| | | |
|------|----------------|--|
| File | New | Start a new scenario — clear input in all data groups |
| | Open | Open an existing scenario <*.scn> file |
| | Save | Save the current scenario file using the previously given name, or the default name <wqnew.scn> |
| | Save As... | Save the current scenario file and specify its filename |
| | Exit | Exit the WAQ-GUI |
| | Visualise area | The visualisation area is a tool for displaying objects bound to a geographical location. This tool is present in several Delft3D models. In the WAQ-GUI, it can be used for visualisation, addition and modification of discharge locations, observation points and open boundaries. For a visual reference, the original hydrodynamic grid is displayed. |
| Help | Contents | Opens the general help menu of D-Water Quality |
| | About | Displays the version number of the GUI |

5.3.1 Description

In the Data Group *Description* you can specify three lines of meta-information about the calculation (Figure 5.17).

The individual text boxes have a length of 39 characters each. Specifying longer text strings seem possible, but the text exceeding 39 characters will be truncated and will not be saved.

5.3.2 Hydrodynamics

In the Data Group *Hydrodynamics* you can specify which coupled hydrodynamic file(s) should be used in the water quality calculation.

From top to bottom, the following four frames can be distinguished (Figure 5.18):

- ◇ Hydrodynamics and grid
- ◇ Time information
- ◇ Horizontal and vertical aggregation
- ◇ Domain decomposition

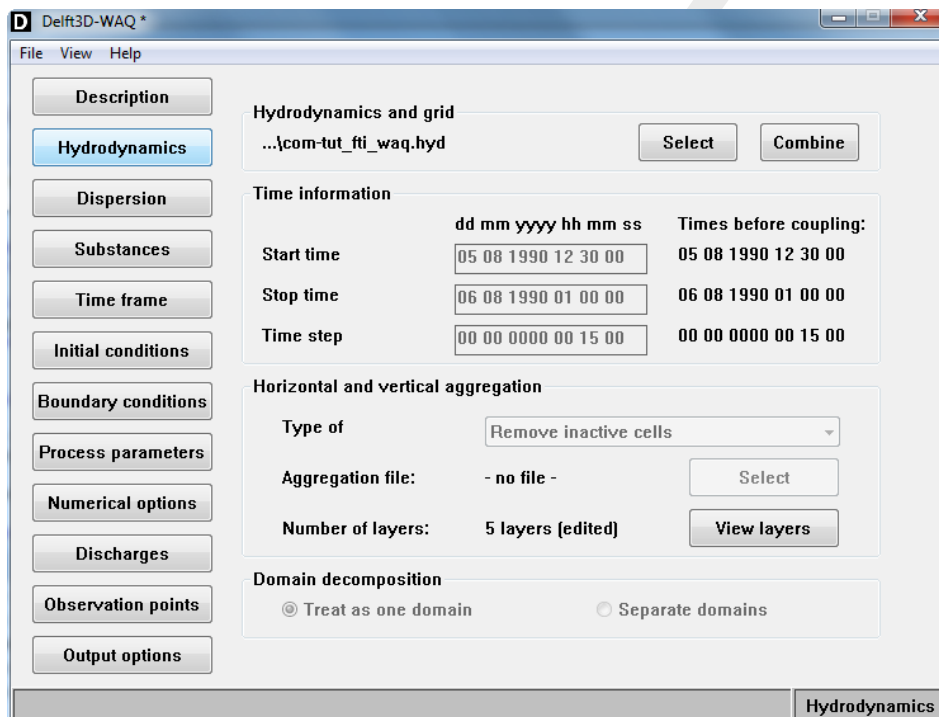


Figure 5.18: Data Group Hydrodynamics

Hydrodynamics and grid

In this frame you can either *Select* a single coupled hydrodynamic file <*.hyd>, a previously generated multiple hydrodynamics file <*.mhy> or generate a multiple hydrodynamic file <*.mhy> using the *Combine* button.

By clicking *Select* you can browse to the right file and press *OK* in the file dialogue for confirmation. By pressing *Combine* you can build a new combination of hydrodynamic files without running Delft3D-FLOW. This option can be very useful, for example if you want to model different seasons that are represented by two different hydrodynamic calculations, in one water quality calculation. Details about combining hydrodynamics can be found in the *Intermezzo*.

The hydrodynamic description file contains almost all the information the user-interface needs to deal with the hydrodynamic database. This includes:

- ◇ *The type of grid:*
The user-interface currently supports two types of hydrodynamic grids, regular curvilinear grids (with or without horizontal aggregation) or so-called unstructured or finite-element grids. This latter type of grid must consist of triangles, by far the most common type for

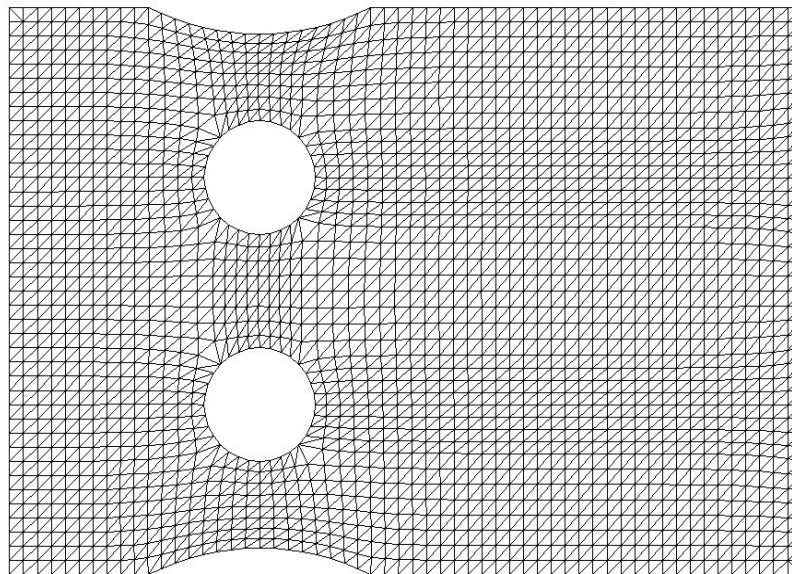


Figure 5.19: Example FEM grid

finite-element grids. (Another aspect of the grid is the type of vertical layers. For details see [section 11.4](#))

◇ *Single domain or multiple domains:*

Most information to be defined for the water quality computation will hold for all domains as a whole, but some data, notably initial conditions may be given *per domain*. It is up to the user-interface to make sure that the computation is started for all domains at once.

◇ *Time information:*

The water quality computation must refer to the correct times in the hydrodynamic database, both in case of a single database and in case of a combination of databases.

◇ *Other information:*

The hydrodynamic description file also contains a list of waste loads and their locations, as found in the hydrodynamic database, the names of the files that constitute this database and so on. All this information is needed at some point or other.

Finite-element grids

The actual coupling to unstructured or finite-element grids is done outside the Delft3D suite itself at the moment. But the hydrodynamic description file is used to pass all the necessary information to the graphical user-interface. Here are the specifics about this type of grid:

- ◇ The keyword grid-type must be set to “finite-elements”.
- ◇ As there is no distinction in two horizontal directions possible, the user-interface presents a single value for determining the location of boundaries and of waste loads and observation points.
- ◇ The visualisation area is adapted to show this type of grid, as well as show the location of special points and boundaries (see [Figure 5.19](#)).

Time information

Details specified in the *Time information* frame are derived from the selected hydrodynamic file and are visualised for information purposes only. Changes to (coupled hydrodynamic) time step, start and stop times can not be made here. The Data Group *Time frame* deals with the specification of the timers in the water quality calculation.

Horizontal and vertical aggregation

Displays the horizontal aggregation that is applied in the selected (coupled) hydrodynamic file. No changes to the horizontal aggregation can be made in the WAQ-GUI. If you want to change the horizontal aggregation, you will have to return to the Coupling routine (Section 5.2.1).

Displays the vertical aggregation that is applied in the selected hydrodynamic file. No changes to the vertical aggregation can be made in the WAQ-GUI. If you want to change the vertical aggregation, you will have to return to the Coupling routine ([section 5.2.1](#)).

Intermezzo: Combining hydrodynamics

D-WAQ allows you to base a water quality simulation on more than one (coupled) hydrodynamic simulation. There are two options to combine hydrodynamic results:

- ◇ Chaining of hydrodynamic results: use one hydrodynamic result during one period and another during the following period.
- ◇ Interpolation of hydrodynamic results: use two (or more) hydrodynamic results during the same period, for instance to get a smooth transition between two periods.

The combination of hydrodynamic results to describe the movement of water over a prolonged period is usually a substitute for a hydrodynamic simulation over that complete period. Generally, a hydrodynamic simulation over a long period (say one year) takes an unrealistically long computation time. An alternative is to choose two or more (hydrodynamically) representative periods that take much shorter computation time, and to interpolate between these representative periods for the rest of the total period.

Representative periods can be distinguished by:

- ◇ River discharges (annual minimum, annual average and annual maximum)
- ◇ Wind speed and direction (typical for monsoon regions with alternating wind directions during the wet and the dry seasons)
- ◇ Spring tide versus neap tide

Be aware that combining hydrodynamic results can never replace actual hydrodynamic modelling; it is no more and no less than a surrogate.

Chaining hydrodynamic results

Suppose you want to do a calculation that covers two or more seasons, a period of six months. One, rather inconvenient way to do this, is to run the hydrodynamic model for this period of six months. This will give a huge data set <com-*.dat>, will probably take a long time to finish and maybe the hydrodynamic model will calculate the same typical flow field for several months and only then switch to another flow field. The alternative is to do a short calculation for the first season, of say two days, and another short calculation for the second season, also two days.

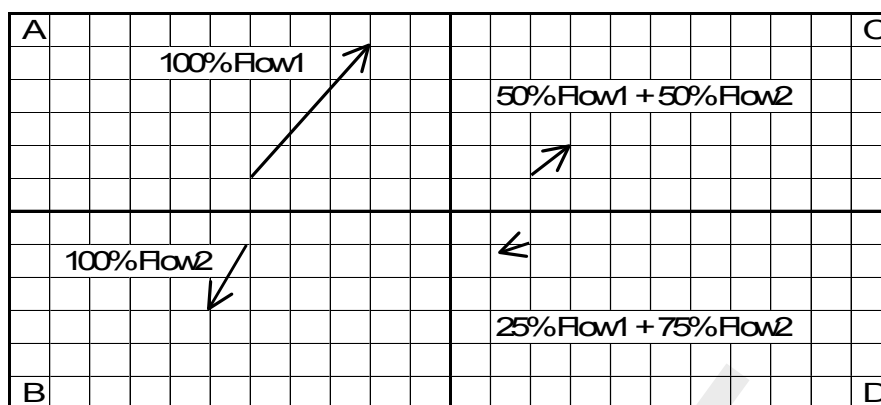


Figure 5.20: Interpolation of flow fields. A) Flow 1 – angle 53° , length 5.00; B) Flow 2 – angle 243° , length 2.24; C) 50 % Flow1 + 50 % Flow2 – angle 45° , length 1.41; D) 25 % Flow1 + 75 % Flow2 – angle 198° , length 0.79.

D-WAQ then allows you to say:

- ◇ Use the first result during the first three months
- ◇ Use the second result during the second three months

Just as with a single hydrodynamic result, D-WAQ will rewind the coupled hydrodynamics files if it reaches their end, before the end of the water quality calculation. It will continue to use (and thus rewind if necessary) the first result until the beginning of the new period.

It is preferable to include a transition period, during which the flow field can adjust relatively smoothly. This is where the second type of combination becomes important.

Interpolation between hydrodynamic results

Interpolation of hydrodynamic results is straightforward. Interpolation is linear and takes into account a weight factor as demonstrated in Figure 5.20.

As mass conservation needs to be preserved, the option for interpolating the flow fields is limited: you can superimpose any number of flow fields, as long as the weighting factors are constant. So a transition period of three days as in the above example might be specified as:

- ◇ The flow field during the first day is 75 % of the first result and 25 % of the second.
- ◇ The flow field during the second day is 50 % of the first result and 50 % of the second.
- ◇ During the third day it is 25 % of the first result and 75 % of the second.

This is illustrated in Figure 5.21.

The weight factors should add up to 100 %. There is no limitation on the number of hydrodynamic results used in the interpolation. In fact, you can use several flow fields for simulating special effects, like:

- ◇ The first result is the flow field without wind
- ◇ The second is the result with a wind speed of 10 m/s

Combining the two via the following formula allows you (under simplified assumptions) to

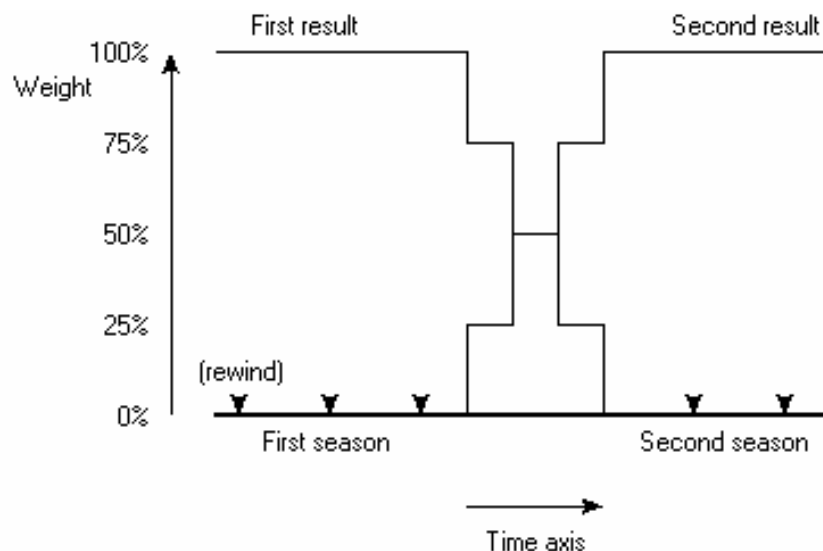


Figure 5.21: Schematic representation of combining hydrodynamic results.

estimate the flow field under any wind speed:

$$\begin{aligned}\text{New flow field} &= \text{first flow field} + \text{factor} \times (\text{second flow field} - \text{first flow field}) \\ &= (1 - \text{factor}) \times \text{first flow field} + \text{factor} \times \text{second flow field}\end{aligned}$$

Adding a third flow field that contains the effect of, say, a large river will make further combinations possible. *Note that the fact that such combinations are logically possible, does not mean that they are physically realistic.*

Hydrodynamic results can be combined only if they are based on the same water quality grid:

- ◇ The underlying hydrodynamic grid must be the same.
- ◇ The layers must have the same (relative) thicknesses and the number of layers must be the same.
- ◇ If horizontal aggregation is applied, this must be the same for all results.
- ◇ The open boundaries must be the same.
- ◇ The discharges that have a flow rate in the hydrodynamics will have to be handled in a special way: it is very cumbersome for you to specify the flow rates and concentrations properly (see the section Treating discharges).

Of course the transition from one period to the next must be smooth enough, for instance, the transition occurs during the time of high water, so that any differences in water level are minimal in terms of the total water depth. To achieve that it is possible to shift the time frame in the hydrodynamic results (see the section Adjusting time frames).

The user-interface takes care of most of the details:

- ◇ After clicking *Combine* in the *Hydrodynamics* Data Group, a dialog appears (see [Figure 5.22](#)).
- ◇ You will select one or more hydrodynamic results for each period.
- ◇ Each result is assigned a weighting factor and an offset in the results file (normally zero, see the section Adjusting time frames).

- ◇ The user-interface checks that the hydrodynamic results are based on the same grid and determines a default calculation period from the given periods. For these checks the first selected hydrodynamic result is used.

Combine hydrodynamic results

Combination option:

| Simulation start time dd mm yyyy hh mm ss | Simulation stop time dd mm yyyy hh mm ss | Hydrodynamics | Scale factor | Offset in file dd mm yyyy hh mm ss |
|--|---|-------------------------|--------------|---------------------------------------|
| 05 08 1990 12 30 00 | 06 08 1990 01 00 00 | ...\com-tut_fti_waq.hyd | 1 | 05 08 1990 12 30 00 |
| 06 08 1990 01 00 00 | 10 08 1990 00 00 00 | ...\com-tut_fti_waq.hyd | 0.5 | 06 08 1990 01 00 00 |
| 06 08 1990 01 00 00 | 10 08 1990 00 00 00 | ...\com-tut_fti_waq.hyd | 0.5 | 06 08 1990 01 00 00 |
| 10 08 1990 00 00 00 | 15 08 1990 00 00 00 | ...\com-tut_fti_waq.hyd | 1 | 10 08 1990 00 00 00 |

New period New hyd-file Delete Re-read Cancel

Figure 5.22: Combining hydrodynamic results. Four periods are defined.

In this dialogue the buttons have the following meanings:

- New period* Create a new period for which a hydrodynamic file <*.hyd> can be selected.
- New hyd file* Add a hydrodynamic file <*.hyd> to the period that is being edited. The start time and stop time will be the same as the first hydrodynamic file <*.hyd> that belongs to this period.
- Delete* Remove the selected record. If there is only one record left for this period, then the period is removed as well.
- Re-read* Exit the **Combine hydrodynamic results** window and save the combined hydrodynamics information.
- Cancel* Exit the **Combine hydrodynamics results** without saving the combined hydrodynamics information.



Remarks:

- ◇ Because a lot of other information depends on the selection of the hydrodynamic result, you should first close the dialogue before doing anything else in the user-interface.
- ◇ The simulation start and stop times shown in Figure 5.22 are the times after coupling.

The list of hydrodynamic results is stored in a file with the extension <*.mhy>. This file can be used as if it were an ordinary hydrodynamic description file. It can be selected via the *Select* button in stead of a <*.hyd> file, but it can not be selected in the combination dialogue, as this would lead to a nested list of hydrodynamic results.

Adjusting time frames

You can shift the hydrodynamics in time. For this the offset time is used. An example may clarify this. Suppose the high water in a spring tide occurs at 2 o'clock in the afternoon, whereas the high water in a neap tide occurs at noon. If you combine these two tidal cycles to estimate the transition from spring tide to neap tide, then you would like to get matching

phases. In other words: the cycle for neap tide must be shifted backwards by 2 hours or the cycle for spring tide must be shifted forwards by 2 hours to get a match. This is done by specifying the offset time as either +2 or -2 hours.

Treating discharges

One final remark must be made about the treatment of discharges defined in the hydrodynamic calculations. When dealing with a single hydrodynamic result, the discharge rates are taken from the hydrodynamic result files and displayed as an ordinary time-series initially defined over the same period as the hydrodynamic result. Beyond that time interval, the discharge pattern is repeated as long as necessary.

To get an equivalent definition with multiple hydrodynamic results the user-interface would have to interpret the specified multiple hydrodynamics and create a time-series that fills the entire period covered by that specification. For instance: during the first season in the previous example the discharge is defined over a period of two days by 10 breakpoints. This pattern should then be repeated until the transition period, so three months later, because only then a different pattern becomes necessary. The user-interface would construct a time-series of 450 breakpoints for these first three months.

So, rather than have the user-interface construct a time-series that covers the complete period, a different approach is chosen:

- ◇ The user-interface constructs a time-series consisting of two breakpoints only: the first time and the last time of the period for which the hydrodynamic results are defined. The flow rate is set to the special value -999.0.
- ◇ The computational program interprets this special value as an instruction to derive the instantaneous flow rate from the flow field directly.
- ◇ You need to specify the concentrations only — at breakpoints that are independent of the hydrodynamics.
- ◇ You are free to change the flow rate. This new flow rate will be used to calculate the amount of substance to be added, but be aware that the original flow is still part of the hydrodynamic flow field and thus will be responsible for taking out mass.

5.3.3 Dispersion

In the Data Group *Dispersion* you can specify the horizontal and vertical dispersion.

From top to bottom, the following three frames are visible ([Figure 5.23](#)):

- ◇ Uniform dispersion
- ◇ Additional vertical diffusion
- ◇ Dispersion arrays

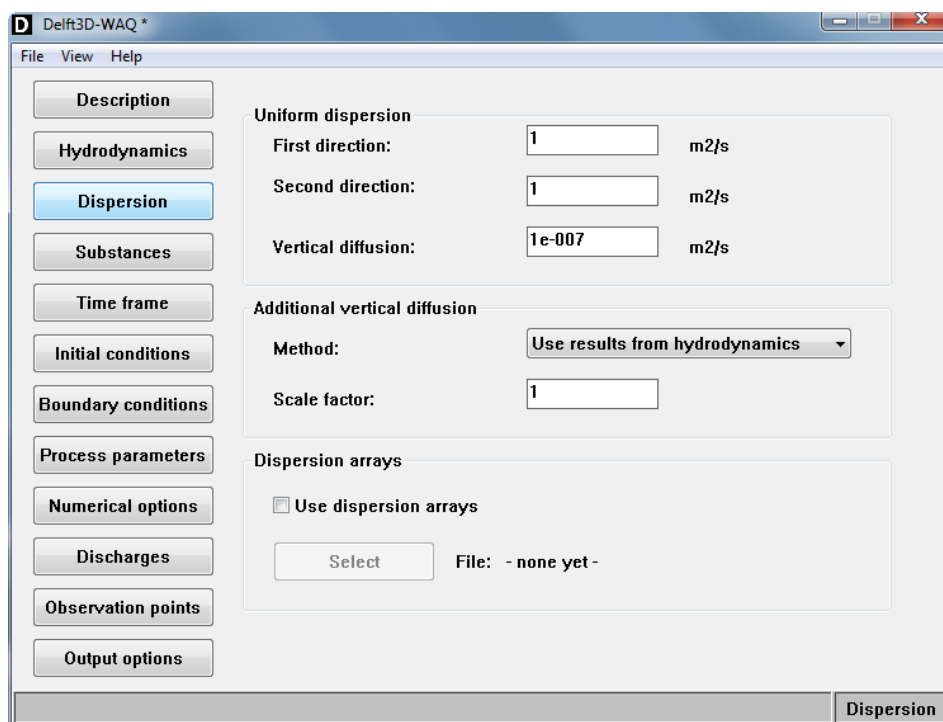


Figure 5.23: Dispersion window

Uniform dispersion

Dispersion coefficients are required to solve the advection-dispersion-equation. Initially, default values are given, but these values can be adapted. In case of a 2D calculation, only the horizontal (i.e. first and second) directions can be edited. To define the 'first' and 'second' direction you should open the visualise area to display the simulation grid. By moving the mouse, the M and/or N values (right upper corner) change. Moving the mouse from bottom to top changes the M-values. This is the 'first' direction. Moving the mouse from left to right changes the N-values. This is the 'second' direction. The third direction (only valid in 3D calculations) is the vertical direction and is not visible in the visualisation area.

It is very unusual to take a different value in the 1st and 2nd direction.

Additional vertical diffusion

If you select the option *Use results from hydrodynamics*, the vertical diffusion derived from the hydrodynamic simulation will be used. This value will be added to the value specified in the uniform dispersion for the third direction. A scale factor can be applied as well.

The option *No additional diffusion* indicates that only the uniform vertical dispersion will be used.

Dispersion arrays

Dispersion values are valid for all exchanges. If you want to exclude a number of exchanges or define a specific dispersion value for a specific region, you can define a so-called 'dispersion array'. A dispersion array is defined with an ASCII-file containing the overridings (exceptions) of the uniform dispersion value. Both exchange number and dispersion value should be specified. The ASCII-file should have the extension <*.dsp>. Use semi-colons (;) to separate the values from comments. The file content is as follows:

```
2           ; 2 = option "additional dispersion with default"
1.0  5.0    ; scale factor and default dispersion in the first direction
3           ; number of overridings in the first direction
exchange_#1 new_dispersion_value
exchange_#2 new_dispersion_value
exchange_#3 new_dispersion_value
1.0  5.0    ; scale factor and default dispersion in the second direction
2           ; number of overridings in the second direction
exchange_#4 new_dispersion_value
exchange_#5 new_dispersion_value
```

Refer to the file description in [section A.2.3](#) on how to retrieve the exchange numbers.

5.3.4 Substances

In the Data Group *Substances* you specify the state variables (modelled substances), the water quality processes and output parameters ([Figure 5.24](#)).

You click *Select* and browse to a substance file <*.sub>, which was created with the PLCT (Processes Library Configuration Tool, refer to [section 5.1](#)). This file contains all relevant information about the substances, processes, parameters and output of the water quality simulation.

Changes to state variables, output parameters, etc. can not be made in this data group. For any changes you will have to return to the PLCT, make the desired changes and reopen the <*.sub> in the WAQ-GUI. The frames *Substances in calculation*, *Output parameters* and *Active processes* are displayed for reference purposes only.

5.3.5 Time frame

The start time, stop time and time step of the water quality simulation are defined in the Data Group *Time frame*.

The *Time frame* Data Group has two frames ([Figure 5.25](#)):

- ◇ *Times in coupled hydrodynamics*
- ◇ *Times in water quality calculation*

Times in coupled hydrodynamics

The times from the coupled hydrodynamics are displayed for reference purposes only and can not be edited.

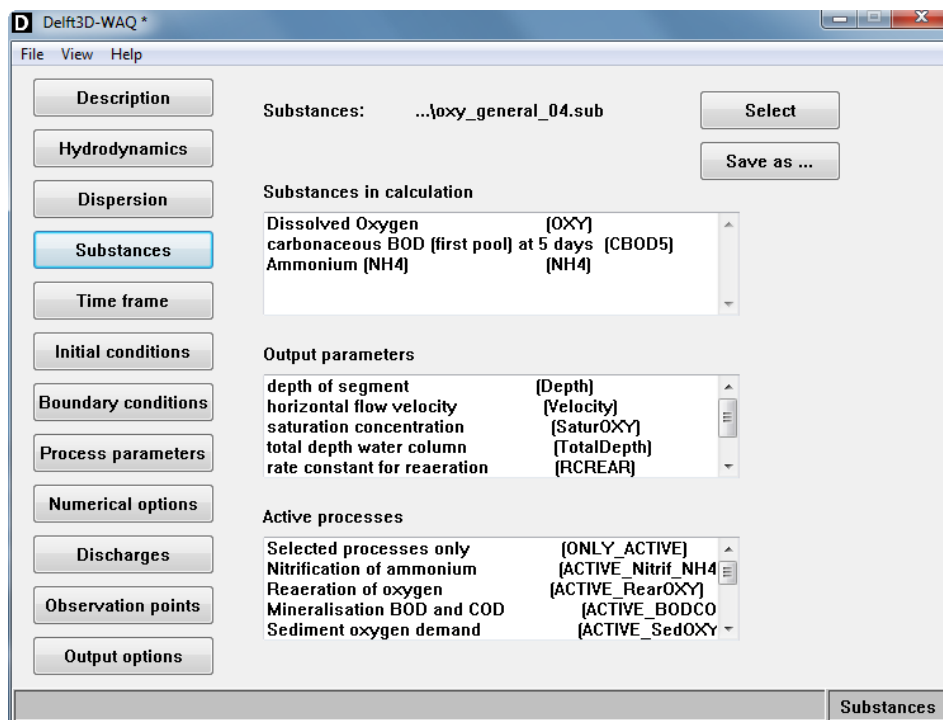


Figure 5.24: Substances Data Group. The standard substance file for dissolved oxygen <oxy_general_04.sub> was selected

Times in water quality calculation

Timers in D-WAQ always have the format 'dd mm yy hh mm ss', or day - month - year - hour - minute - second. The start time, stop time and time step of the water quality simulation have to satisfy these conditions:

- ◇ The start time of the water quality simulation has to be equal to or later than the start time in the coupled hydrodynamics.
- ◇ The stop time of the water quality simulation has to be later than the start time in the water quality simulation.
- ◇ The time step in the water quality simulation has to be equal to or an integer division of the time step in the coupled hydrodynamics. So if the time step in the coupled hydrodynamics is 15 minutes, the time steps allowed in the water quality simulation are 15 minutes, 7.5 minutes, 5 minutes, etc.
- ◇ The minimum time step allowed is one 1 second.
- ◇ The total time between the start time and the stop time in the water quality simulation has to be an integer multiplication of the time step in the water quality simulation.

The WAQ-GUI will check if the specified start time, stop time and time step comply with these conditions when you exit the *Time frame* Data Group or when you click *Time frame*.

Note that it is allowed to extend the water quality simulation beyond the stop time of the coupled hydrodynamics. D-WAQ will rewind and repeat the coupled hydrodynamics as often as required to cover the time period specified. As explained in Section 4.1.1 you have to take care that no extreme transition in for example water level occur as a result of the rewinding.



Remarks:

- ◇ When setting up a scenario from scratch, the start and stop times of the simulation period will be used as defaults for the start and stop times in time-series for boundaries,

The screenshot shows a window titled 'Data Group Time frame' with two main sections:

- Times in coupled hydrodynamics**
 - Start time: 05 08 1990 12 30 00
 - Stop time: 06 08 1990 01 00 00
 - Time interval: 00 00 0000 00 15 00
 - Reference time: 05 08 1990 00 00 00
- Times in water quality calculation**
 - Header: dd mm yyyy hh mm ss
 - Start time: 05 08 1990 12 30 00
 - Stop time: 15 08 1990 00 00 00
 - Time step: 00 00 0000 00 15 00

Figure 5.25: Data Group Time frame

process parameters, discharges and output period. This holds as long as you do not specify timings yourself.

- ◇ When changing the start or stop time in an existing scenario, the start and stop time of other time-series or output period are not adjusted.
- ◇ The water quality time frame may not differ more than 5 years from the hydrodynamic time frame.

5.3.6 Initial conditions

Initial conditions are the concentrations of substances at the start of the simulation. By default they are all zero. Initial conditions have to be specified for all substances that are included in the substances file <*.sub>. Note that as long as no substance file <*.sub> has been selected this window will be empty.

The *Initial conditions* Data Group contains a list of substances and entry boxes in which a constant initial concentration can be specified simply by typing an entry. Always make sure that the units are correct.

At the bottom of the data group there are two buttons:

- ◇ *Edit data*
- ◇ *Information*

In case you want to specify non-constant initial conditions you have to use *Edit data*. Non-constant conditions are spatially varying such as a salinity field or temperature profiles. Non-constant initial conditions have to be specified for every computational cell and are therefore usually derived from secondary input files.

When selecting an edit field, the value can be edited by directly typing or clicking *Edit data*. The latter opens the **Data for:** <substance> window (Figure 5.27). The following menu items are available (menu-item *Help* is not explained here):

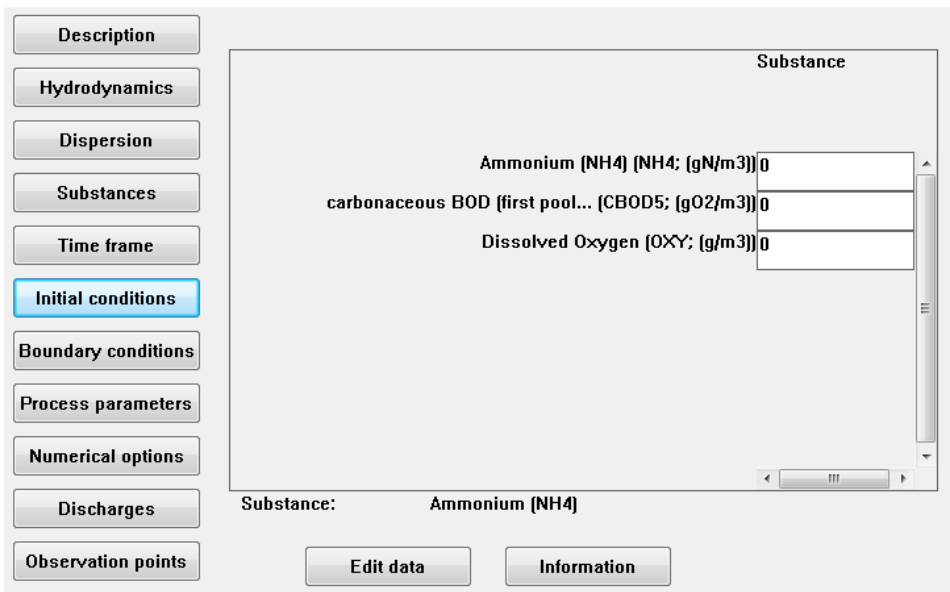


Figure 5.26: Data Group Initial conditions. By default all concentrations are set to zero.

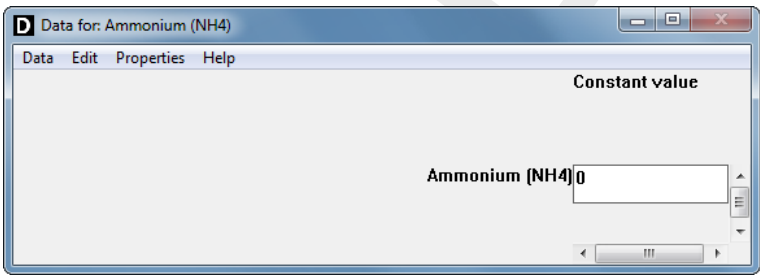


Figure 5.27: Data for: <substance> window opened for Ammonium. A constant value can be specified

| | | |
|------------|---------------|---|
| Data | Import... | Select a secondary file to import initial conditions; the Import data file window is opened. |
| | Quit | Closes the Data for: <substance> window without saving changes; a confirmation is asked. |
| | Save and exit | Closes the Data for: <substance> window and saves the input. |
| Edit | (no options) | |
| Properties | Details | Opens the Details for quantity window (Figure 5.28) in which you can specify whether the initial condition is a constant value or a scalar field (i.e. spatially varying). In case of the latter a data file has to be imported using the <i>Data</i> → <i>Import...</i> item. |

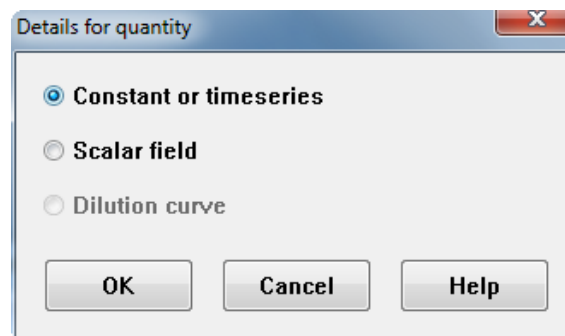


Figure 5.28: *Details for quantity* window for selection between constant or spatially varying initial conditions

Import data file

Non-uniform values (i.e. a scalar field) are imported from an external file. The following types are allowed:

- ◇ QUICKIN data file (<*.qin>)
- ◇ QUICKIN 3D data file (<*.q3d>)
- ◇ D-WAQ map file (<*.map>)
- ◇ D-WAQ (NEFIS) map file (<*.ada>)
- ◇ D-WAQ segment function (<*. *>)

For a detailed definition of the files refer to [Appendix A](#). QUICKIN (QUICKIN UM, 2013) is a Delft3D software package that is used to generate the bathymetry for hydrodynamic simulations. However, you can use it to generate a non-uniform parameter field as well. QUICKIN files are generated on the (non-aggregated) hydrodynamic grid and can be used in all water quality simulations based on this hydrodynamic grid. If an aggregated grid is used in the water quality simulation, values will be aggregated through simple averaging.

The D-WAQ map files (<*.map> and <*.ada>) are output files from a previous simulation. They can only be used if the grid is identical: the grid of the map file has to match the grid in the current water quality simulation. An error message is displayed if this is not the case.

Remark:

- ◇ A 2D WAQ map file can be used as initial condition for a 3D model if the horizontal grid is the same.



Finally, the D-WAQ segment function is a binary file with values for all computational cells. Water temperature <*.tem>, salinity <*.sal>, shear stress <*.tau> and vertical diffusion <*.vdf> can be derived from the hydrodynamic simulation and are examples of segment functions. Also, segment functions can be prepared with simple programs (see [Appendix A](#)).

Use the *File type* dropdown box to specify the right type and click *Select* for browsing to and selecting the file. After opening the file, the window looks as displayed in [Figure 5.29](#).

Subsequently, specify the desired parameter and time (map files and segment functions can have more than one time step). The corresponding values will be 'extracted' from the file after pressing *Import*. The edit field behind the substance is now indicating '[from file]'. To review which file was selected, return to the **Import data file** window.

If you click *Import all*, the WAQ-GUI will compare the substances with the available information

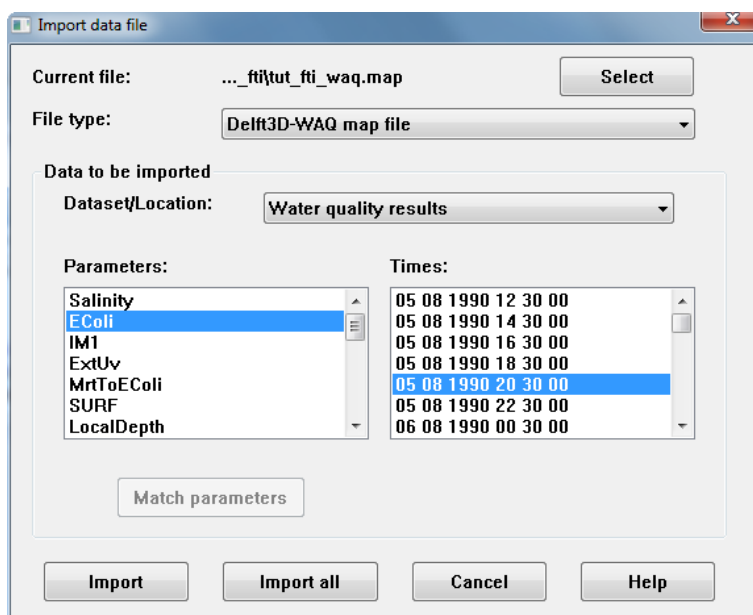


Figure 5.29: Import data file window. A D-WAQ map file <*.map> is selected. The Ecoli concentration on August 05, 1990 20:30 will be used as initial condition

in the selected file and initial conditions will be set for all substances for which a matching name is found in the selected file. This prevents unnecessary repetition of actions in case you have to set the initial condition for a lot of substances.

A special type of <*.map> file is the restart file <*_res.map> in which the concentration of all substances on the final time step of the water quality simulation are stored. The restart file <*_res.map> can be used too as initial condition for a new simulation. This might be especially useful in cases where the spin-up time of the model is long.

Ranges and typical values

For informative purposes the *Information* button opens the **Ranges and typical values** window. It gives a range of values for each of the substances (if available). The values of around 20 common substances are stored in an internal Delft3D file <watqual.d3d> and will be available after installing D-Water Quality. These values can be modified by changing this (internal) file.

5.3.7 Boundary conditions

In this data group you can specify the boundary conditions at the open boundaries of the model grid (outside world). Open boundaries are those boundaries of the model grid that have a cross-section with a non-zero water flow. You have to specify the concentrations of all active substances and they are required for all time steps in the model. No boundary concentrations are needed for the inactive substances as they can not be transported and thus can not enter over the model boundaries. If the stop time of the water quality simulation is later than the last time step for which boundary conditions are specified, D-WAQ will repeat / rewind the time-series from the beginning.

Usually, boundaries are defined in the hydrodynamic simulation and therefore do not need to be redefined in D-Water Quality. Pre-defined boundaries sections might be split in smaller sections if you want to assign different concentrations within a pre-defined boundary section.

| | Typical value | Minimum | Maximum |
|---------------------------|---------------|---------|---------|
| Ammonium (NH4) [(gN/m3)] | - | - | - |
| CBOD5 [(gO2/m3)] | - | - | - |
| Dissolved Oxygen [(g/m3)] | 8 | 3 | 12 |

Figure 5.30: Ranges and typical values window. Values are derived from the <watqual.d3d> file. No information is available for CBOD5

Boundary section: definition

A boundary section is a part of the model boundary for which boundary conditions are uniform in horizontal direction, have the same profile in vertical direction, and have the same time dependency. Boundary sections are defined by giving the grid indices (the (M,N) indices) of the first and last segment of the section. Thus, boundary sections are either sections with a fixed M, but varying N, or vice versa. For aggregated grids, still the grid indices of the original grid are used.

Figure 5.31: Data Group Boundary conditions

The window contains a list of open boundary sections, several buttons at the right-hand side and text boxes displaying the details of the selected boundary section (Figure 5.31).

Restriction:



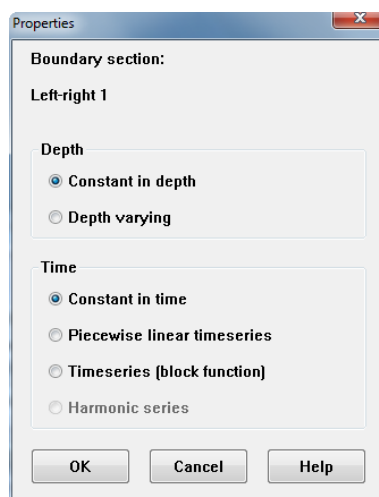


Figure 5.32: Setting **Data properties**. By default boundary conditions are set to 'Constant in depth' and 'Constant in time'

- ◇ The name of a boundary section is restricted to 39 characters.

Editing sections

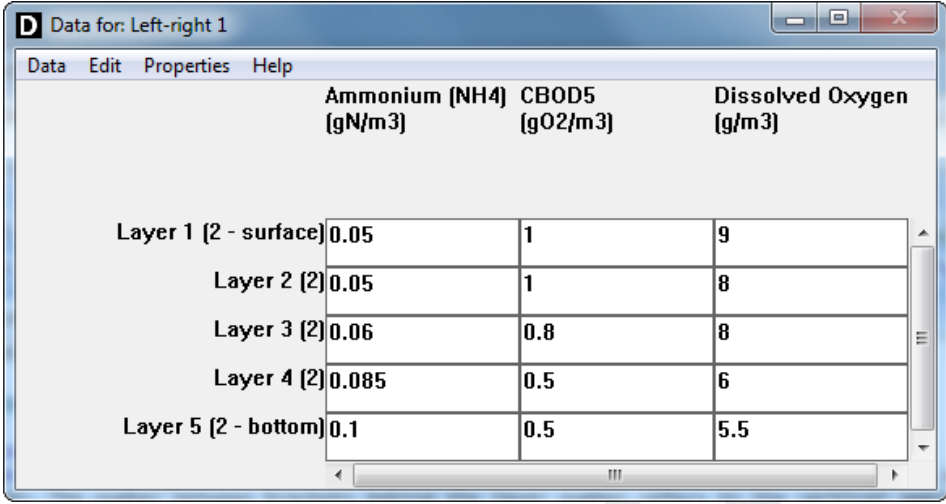
By default, the boundary sections from the hydrodynamics are displayed. If you want to define new boundary sections, press *Add*. Selecting a boundary section and pressing *Delete* will remove that specific section. Pressing *Edit data* will open the **Data for: <Name of boundary section>** window, in which you can specify the concentrations. Pressing *Data file* will open the **Select boundary data file** window, in which you can specify which file will be used for the boundary concentrations, button *Select*. Then you have to check *Use selected file instead of the editable boundary data* to overrule the manual edited data and you have to specify the file format of the chosen file. Pressing *Default sections* will restore the original boundaries derived from the hydrodynamic simulation.

It is compulsory to define concentrations for all boundary sections. The concentration may be zero, but a value has to be specified. Therefore, no entire boundaries or parts of boundaries may be missing. The WAQ-GUI will check whether this condition is fulfilled, when you leave the Data Group *Boundary conditions* or when you press *Boundary conditions*. Boundaries will be restored in case of an error and a warning will be given.

The **Data for: <Name of boundary section>** window in the Data Group *Boundary conditions* is analogous to that in the Data Group *Initial conditions* (Figure 5.27).

The following menu items are available (menu-item *Help* is not explained here):

| | | |
|-------------|----------------------|--|
| <i>Data</i> | <i>Copy...</i> | Copies data from another boundary section. |
| | <i>Import...</i> | Select a secondary file to import boundary conditions; the Import data file window is opened. |
| | <i>Quit</i> | Closes the Data for: <Name of boundary section> window without saving changes; a confirmation is asked. |
| | <i>Save and exit</i> | Closes the Data for: <Name of boundary section> window and saves the input. |



| | Ammonium (NH4) [gN/m3] | CBOD5 [gO2/m3] | Dissolved Oxygen [g/m3] |
|-----------------------|---------------------------|-------------------|----------------------------|
| Layer 1 [2 - surface] | 0.05 | 1 | 9 |
| Layer 2 [2] | 0.05 | 1 | 8 |
| Layer 3 [2] | 0.06 | 0.8 | 8 |
| Layer 4 [2] | 0.085 | 0.5 | 6 |
| Layer 5 [2 - bottom] | 0.1 | 0.5 | 5.5 |

Figure 5.33: Depth varying boundary conditions. A concentration has to be specified for every active substance and every layer. The number between brackets behind the layer number refers to the vertical aggregation.

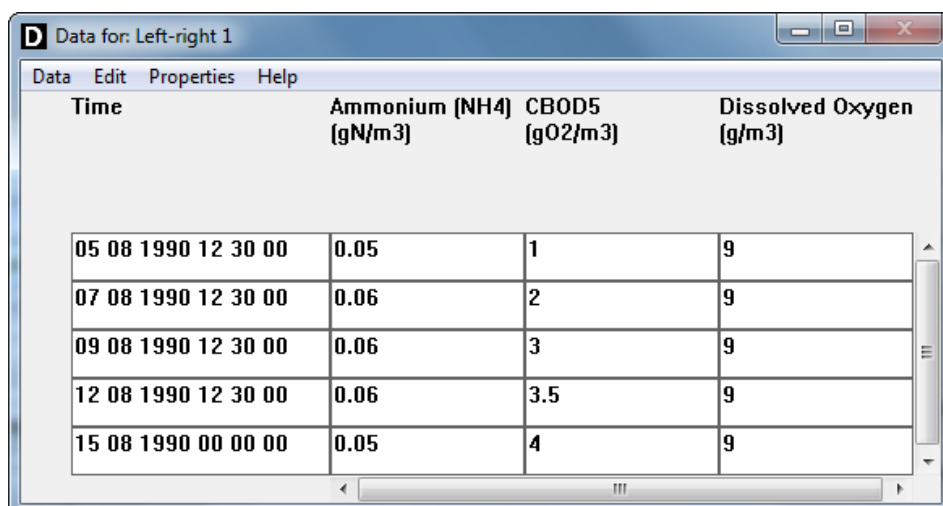
| | | |
|------------|--------------------|--|
| Edit | Copy row or Ctrl+K | Copies the row containing the prompt and put the new row above it in a table. |
| | Delete row | Deletes a row from a table. |
| | Fill column | Copies the selected value into the whole column. |
| Properties | Data properties | You can set two options (Figure 5.32): |
| | | <ul style="list-style-type: none"> ◇ Are the boundary conditions constant in time or varying in time? Variation in time can be as a block function or as a linear function. ◇ Are the boundary conditions constant over depth or varying over depth? |

Setting the boundary conditions to either depth or time varying properties will result in a table in the **Data for: <Name of boundary section>** window. If the boundary conditions are depth varying a boundary concentration has to be specified for every (active) substance and every layer (Figure 5.33). If the boundary conditions are time varying a boundary concentration has to be specified for every (active) substance and every time step (Figure 5.34). Variation in time can be carried out either through linear or block interpolation. Refer to the Intermezzo for an explanation.

Both time and depth varying boundary conditions are not yet supported by the WAQ-GUI. However, it is possible to include both time and depth varying boundary conditions in the input file <*.inp>. An additional manual is available for manual editing of this input file: 'Documentation of the input file, User Manual'. Contact Delf3D-support for information.

Intermezzo: Linear and Block interpolation

Figure 5.35 demonstrates the difference between a linear interpolation of a time-series and a block interpolation. You have to specify time breakpoints (left column in Figure 5.35) and parameter values or concentrations at those time breakpoints (right column in Figure 5.35). For



| Time | Ammonium (NH4) (gN/m ³) | CBOD5 (gO ₂ /m ³) | Dissolved Oxygen (g/m ³) |
|---------------------|--|---|---|
| 05 08 1990 12 30 00 | 0.05 | 1 | 9 |
| 07 08 1990 12 30 00 | 0.06 | 2 | 9 |
| 09 08 1990 12 30 00 | 0.06 | 3 | 9 |
| 12 08 1990 12 30 00 | 0.06 | 3.5 | 9 |
| 15 08 1990 00 00 00 | 0.05 | 4 | 9 |

Figure 5.34: Time varying boundary conditions. A concentration has to be specified for every active substance and every time step. The number between brackets behind the layer number refers to the vertical aggregation. The type of interpolation (linear or block) can be reviewed through the Properties → Data Properties

linear interpolation the parameter values or concentrations in between the time breakpoints are calculated based on a linear average between the two adjacent time breakpoints. In case of block interpolation, the parameter value or concentration remains constant until the next time breakpoint and then instantly changes to the new value.



Remarks:

- ◇ If the stop time of the water quality simulation is later than the last time breakpoint in the time-series, the time-series will be repeated from the first time breakpoint (rewinding occurs).
- ◇ Note that in block interpolation the last time breakpoint is not used.

Visualisation Area

The Visualisation Area (VA) can be opened to view the location(s) of the boundary section(s). Select the menu-option *View* → *Visualise area* for opening the VA. You can also use the VA for defining new sections. A section can be defined by drawing a line with your mouse from the first to the last segment of the section. Boundary sections appear with a red colour. Note that if you create a new boundary section, you have to delete some segments from another section since every segment can be defined only once.

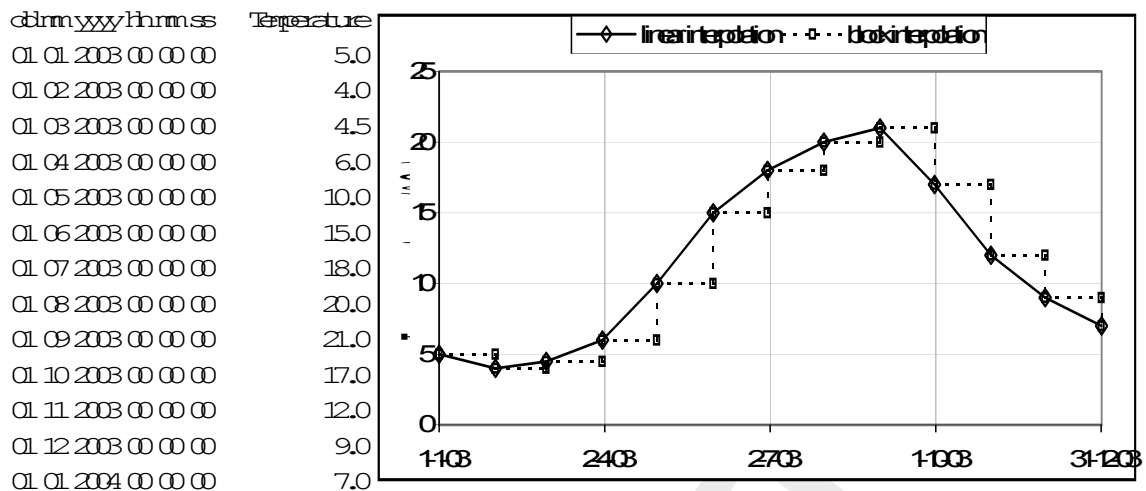


Figure 5.35: Difference between linear and block interpolation of a time-series of water temperature in 2003

Timelag

The edit field *Time lag* allows you to specify a time lag for the selected boundary section. This time lag uses a Thatcher-Harleman transition to smooth the transition between inflow and outflow on boundaries. The time lag is given in the format “dd mm yyyy hh mm ss”, as for all date/time values. Refer to Section 8.5 for more information on the Thatcher-Harleman time lag.

Boundary conditions may have an important effect on the final model results. Therefore, the model grid schematisation should be large enough to prevent any unwanted concentration fluctuations resulting from these boundaries, or from irregularities in the hydrodynamic flows across these boundaries. In case the boundaries are far away from the area of interest (a discharge location, an estuary, a harbour, a regional sea, etc.) it usually suffices to take constant boundary conditions (obviously, the constant values should be chosen carefully). However, for studies over longer periods of time, time-dependent boundary conditions are still required. Probably, you will have to specify different boundary conditions for all default boundary sections. Default boundary sections are not adjacent and may have very different flow and concentration distributions. Pressing *Default sections* will restore the original number of boundary sections and set the properties of each back to ‘constant in depth’ and ‘constant in time’.

5.3.8 Process parameters

In this data group you can specify the process parameters which are available through the selected substance file <*.sub>. A listing of available parameters is shown in Figure 5.36.

By default the process parameters will be constant in time and space. However, process parameters can vary in time and/or space. Initially process parameters will have the default value that is taken from the PLCT. These values may be altered in the *Process parameters* Data Group. When you select a new substance file <*.sub> in the Data Group *Substances*, identical process parameters will not be overwritten with the default values and therefore information will be conserved. Obviously, process parameters that are new in the substance file <*.sub> will be added to the list with their default value.

In some occasions the default value may be ‘-999’ which is interpreted as a missing value. You have to specify a value in order to activate the process(es) that uses this value.

Process parameter

ambient water temperature [Temp; [oC]]

(timeseries)

first-order nitrification rate [RcNit; [1/d]]

0.1

decay rate BOD (first pool) ... [RcBOD; [1/d]]

0.3

critical oxygen concentratio... [COXBOD; [gO2/m3]]

1

optimum oxygen concentration... [OOXBOD; [gO2/m3]]

5

Salinity [Salinity; [g/kg]]

- to be imported -

wind speed [VWind; [m/s]]

3

switch for oxygen reaeration... [SWRear; [-]]

1

Process parameter: first-order nitrification rate

Edit data

Figure 5.36: Data Group Process parameters. A time-series is specified for the water temperature, a segment function for salinity. All other process parameters have constant values

Importing of time-series <*.tim> will automatically adjust the properties.

Editing data

By selecting an edit field and pressing *Edit Data* the **Data for: <substance name>** window appears. The following options are available (menu-item *Help* is not explained here):

| | | |
|------------|-----------------|--|
| Data | Import... | Select a secondary file to import parameter values; the Import data file window is opened. |
| | Quit | Closes the Data for: <substance name> window without saving changes; a confirmation is asked. |
| | Save and exit | Closes the Data for: <substance name> window and saves the input. |
| Edit | Copy row | Copies the row containing the prompt and put the new row above it in a table. |
| | Delete row | Deletes a row from a table. |
| | Fill column | Copies the selected value into the whole column. |
| Properties | Data properties | You can set two options (Figure 5.32): <ul style="list-style-type: none">◇ Are the boundary conditions constant in time or varying in time? Variation in time can be as a block function or as a linear function.◇ Are the boundary conditions constant |

over depth of varying over depth?

Details

Opens the **Details for quantity** window ([Figure 5.28](#)) in which you can specify whether the process parameter is a constant value or a time-series or a scalar field (i.e. spatially varying). In case of the latter a data file has to be imported using the *Data* → *Import...* item.

Import data file

Non-uniform values can be imported from an external file. Non-uniform values can be time-series or spatially varying. The following types are allowed:

- ◇ Time-series:
 - Time-series file (<*.tim>) (Note that the name of the process parameter in the <*.tim> file has to match the name in the WAQ-GUI exactly.)
 - Simple locations / table (<*.*)
- ◇ Spatially varying (Scalar field):
 - QUICKIN data file (<*.qin>)
 - QUICKIN 3D data file (<*.q3d>)
 - D-WAQ map file (<*.map>)
 - D-WAQ (NEFIS) map file (<*.ada>)
 - D-WAQ segment function (<*.*)

For a detailed description of the files refer to [Appendix A](#). Use the *File type* dropdown box to specify the right type and click *Select* for browsing to and selecting the file.

QUICKIN is a Delft3D software package that is used to generate the bathymetry for hydrodynamic simulations. However, you can use it to generate a non-uniform parameter field as well. QUICKIN files are generated on the (non-aggregated) hydrodynamic grid and can be used in all water quality simulations based on this hydrodynamic grid. If an aggregated grid is used in the water quality simulation, values will be aggregated through simple averaging.

The D-WAQ map files (<*.map> and <*.ada>) are output files from a previous simulation. They can only be used if the grid is identical: the grid of the map file has to match the grid in the current simulation. An error message is displayed if this is not the case.

Finally, the D-WAQ segment function is a binary file with values for all computational cells. Water temperature <*.tem>, salinity <*.sal>, shear stress <*.tau> and vertical diffusion <*.vdf> can be derived from the hydrodynamic simulation and are examples of segment functions. Also, segment functions can be prepared with simple programs (see [Appendix A](#)).

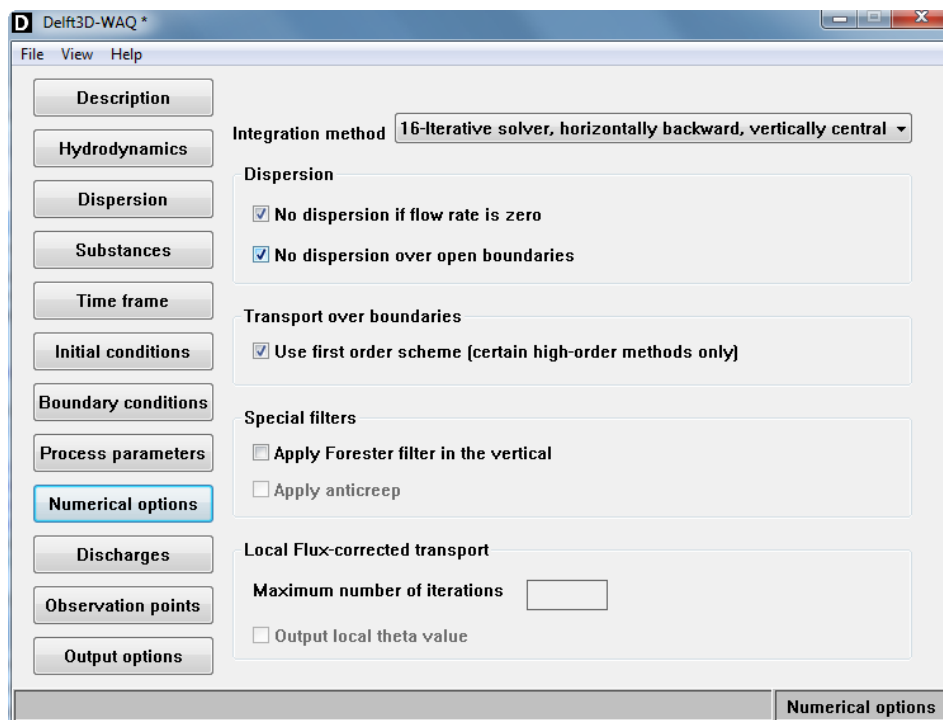


Figure 5.37: Data Group Numerical options

5.3.9 Numerical options

In this data group the numerical scheme to solve the advection-dispersion equation can be selected. The window contains a drop-down box and three frames for defining more detailed numerical options for boundary conditions, dispersion and special filters (Figure 5.37).

You can scroll the *Integration method* drop-down box and you can select the numerical scheme. Time-explicit and time-implicit methods are available. Numerical options also differ in their handling of the vertical direction. In Section 10.5 more information about numerical integration methods can be found.



Remark:

- ◇ If you have merged the multi-domain flow results into a single domain water quality model, numerical schemes 19 and 20 are not allowed.

Numerical options for dispersion

Two options for dispersion are available:

- ◇ No dispersion if the flow rate is zero. It is advised to tick off this checkbox for calculations with tidal flats (areas that can be temporarily dry). Tidal flats require that for zero flow there is no dispersive transport.
- ◇ No dispersion over open boundaries. It is advised to select this checkbox in situations where the boundaries are far away from your area of interest. In other words: preferably the boundary sections should not influence the situation in your area of interest. The (uniform) dispersion coefficient is a system property and is used to calibrate the system. An (additional) dispersion effect over the open boundaries is unwanted in these cases.

Numerical options for transport over boundaries

One option is available for advective transport over the boundaries. It is advised to tick off this checkbox in order to prevent numerical oscillations (boundary reflections) at the boundaries for higher order spatial discretised schemes.

D-WAQ is especially designed for far-field modelling of large systems. In most of these cases these three checkboxes will be ticked off.

Special filter - Forester

The Forester filter (in the vertical) is available for numerical schemes 3, 11, 12, 16 and 19.

It is well-known that second or higher order advective difference methods on coarse grids may exhibit non-physical oscillations near regions of steep gradients. The different numerical schemes do not guarantee positive solutions and consequently negative concentrations may occur. In case of negative concentrations an iterative filter procedure based on local diffusion followed by a vertical filter is started in order to remove the negative values. The filtering technique in this procedure is the so-called Forester filter ([Forester, 1979](#)), a non-linear approach which removes the computational noise without inflicting significant amplitude losses in sharply peaked solutions.

If concentration $c_{m,n,k}$ is negative, then the iterative, mass conservative filtering process is described (for the sake of simplicity only in one direction) by:

$$c_{m,n,k}^{p+1} = c_{m,n,k}^p + \frac{c_{m+1,n,k}^p - c_{m,n,k}^p}{4} \min \left(1, \frac{V_{m+1,n,k}}{V_{m,n,k}} \right) + \frac{c_{m-1,n,k}^p - c_{m,n,k}^p}{4} \min \left(1, \frac{V_{m-1,n,k}}{V_{m,n,k}} \right) \quad (5.1)$$

with $V_{m,n,k}$ denoting the volume of cell (m, n, k) . Only in grid cells with a negative concentration this filter is applied. The superscript p denotes the iteration number. The filter smoothes the solution and reduces the local minima (negative concentrations). [Equation \(5.1\)](#) can be interpreted as an approximation of the following advection-diffusion equation:

$$\frac{\partial c}{\partial t} = \frac{\alpha - \beta}{4} \frac{\Delta x}{\Delta t} \frac{\partial c}{\partial x} + \frac{\alpha + \beta}{4} \frac{\Delta x^2}{\Delta t} \frac{\partial^2 c}{\partial x^2} + \text{higher order terms} \quad (5.2)$$

with:

$$\alpha = \min \left(1, \frac{V_{m+1,n,k}}{V_{m,n,k}} \right),$$

and:

$$\beta = \min \left(1, \frac{V_{m-1,n,k}}{V_{m,n,k}} \right).$$

The Forester filter introduces an artificial advection and diffusion. The numerical diffusion coefficient of the horizontal filter is:

$$D_{num} = \frac{\alpha + \beta}{4} \frac{\Delta x^2}{\Delta t} \leq \frac{\Delta x^2}{2\Delta t}. \quad (5.3)$$

Thus the filter introduces numerical diffusion but only locally. Maximal 100 iterations are carried out. If there is still a grid cell with a negative concentration after 100 iterations, then a

warning is generated. To further understand the influence of the Forester filter, we rewrite Equation (5.1) as:

$$c_{m,n,k}^{p+1} = \left(1 - \frac{\alpha + \beta}{4}\right) c_{m,n,k}^p + \frac{\alpha}{4} c_{m+1,n,k}^p + \frac{\beta}{4} c_{m-1,n,k}^p. \quad (5.4)$$

As both $\alpha \leq 1$ and $\beta \leq 1$ all coefficients of Equation (5.4) are positive. Consequently, a positive concentration will remain positive, i.e. it will not introduce negative concentrations irrespective the steepness of the concentration gradients. A negative concentration surrounded by positive concentrations, usually the result of ill represented steep gradients (wiggles), will be less negative after one iteration and is effectively removed after several iterations by adding enough (local) diffusion to force the concentration to become positive.

Local maxima and minima in temperature or salinity in the vertical direction, generated by the computational method may give physically unstable density profiles and can also better be removed by a numerical filter than by turbulent vertical mixing. A similar filtering technique as in the horizontal direction is applied for points with a local maximum or minimum in the vertical.

Special filter - Anticreep

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; see section 10.6 for details.

The *anticreep* filter can only be used for numerical schemes 19 and 20.

5.3.10 Discharges

In the Data Group *Discharges*, the discharge locations and specific details can be specified.

Figure 5.38 shows a list of discharges and geographical details of the selected discharge at the lower half of the window. At the right-side, four buttons allow you to manage the discharges and import the corresponding data or new discharge locations.

Discharges already present in the hydrodynamic calculation automatically transferred to the water quality simulation and appear in the window with their names; the suffix '(new)' is added to distinguish them. For some discharges a numbered suffix can be added in order to distinguish between various layers. The number between brackets then refers to the number of hydrodynamic layers in the water quality layer.



Restriction:

- ◇ The name of a discharge is restricted to 20 characters.

Discharges can be specified with the use of the Visualisation Area (menu item *View* → *Visualise area*). After opening, use the *Edit* menu for selecting *Discharges* and use the *Edit Mode* for setting the action (*Add*, *Delete*, *Modify*). If you use *Add*, every click within the model area will add a new discharge. Details can be specified in the edit fields in the main window. By selecting *Delete* and subsequent clicking on an existing discharge, the discharge will be deleted. *Modify* means moving the discharge to another location. By selecting this option, you can select an existing discharge, then click a new location within the model grid and the discharge will move to this new location.

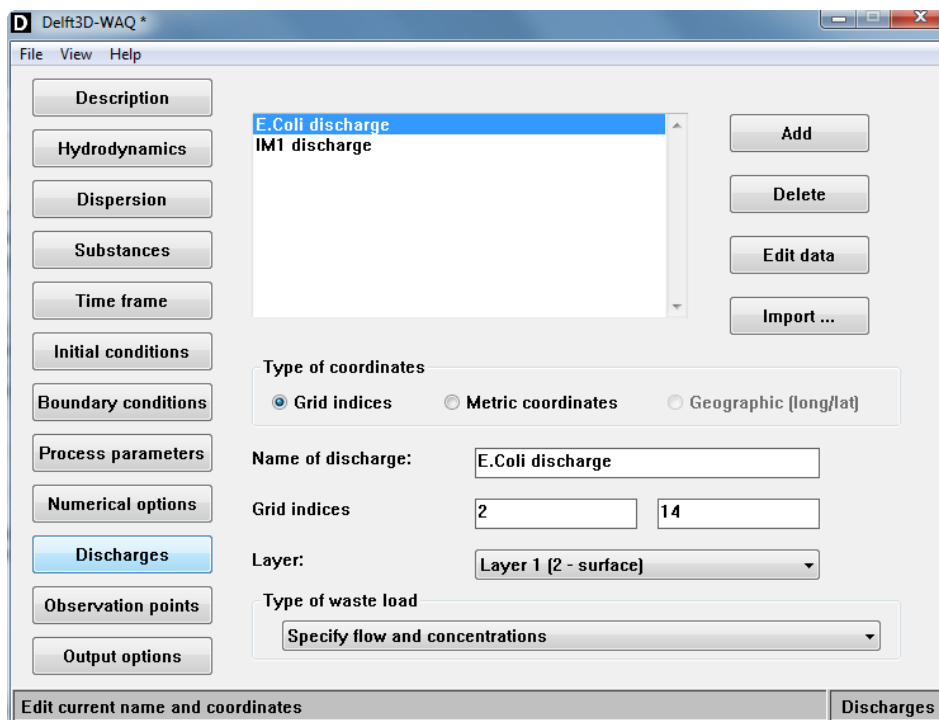


Figure 5.38: Data Group Discharges.

Import data

Data of discharges (location and concentration!) can be imported from a file using the *Import...* option. Data is usually available in a spreadsheet and — when set in the right format — can be directly imported in the WAQ-GUI. Two file types are allowed:

- ◇ Time-series file <*.tim>
- ◇ Simple locations/table file <*.x>

For a detailed description of the file formats refer to [Appendix A](#). The files should contain discharge names, co-ordinates and concentrations or mass loads. Again, concentrations can only be used if the flow rate is not equal to zero. If the flow rate is zero, the value will be interpreted as a mass load.

Edit data

Discharges can also be defined by specification of the grid indices and the layer number by hand. By selecting a discharge in the list box and pressing *Edit data*, flows and concentrations of the discharge can be specified.

The **Data for: <Discharge name>** window contains the following menu items:

| | | |
|-------------|----------------------|--|
| <i>Data</i> | <i>Copy...</i> | Copies data from another discharge. |
| | <i>Import...</i> | Select a secondary file to import parameter values; the Import data file window is opened. |
| | <i>Quit</i> | Closes the Data for: <Discharge name> window without saving changes; a confirmation is asked. |
| | <i>Save and exit</i> | Closes the Data for: <Discharge name> |

| | | |
|-------------------|------------------------|---|
| | | window and saves the input. |
| <i>Edit</i> | <i>Copy row</i> | Copies the row containing the prompt and put the new row above it in a table. |
| | <i>Delete row</i> | Deletes a row from a table. |
| | <i>Fill column</i> | Copies the selected value into the whole column. |
| <i>Properties</i> | <i>Data properties</i> | You can set two options (Figure 5.32): |
| | | <ul style="list-style-type: none">◇ Are the boundary conditions constant in time or varying in time? Variation in time can be as a block function or as a linear function.◇ Are the boundary conditions constant over depth or varying over depth? |

Additional to the concentrations of the substance in the discharge, each discharge has a flow rate (in [m³/s]) as well. Discharges taken from the hydrodynamic simulation always have a non-zero flow rate.

Layer specification

The layer in which the discharge is placed, can be selected in the drop-down box at the bottom of the window. When you select the option *Uniform over depth*, the discharge will be distributed over the complete water column. The discharge will be scaled in accordance with the vertical aggregation. Thus, if three hydrodynamic layers are aggregated to two water quality layers (depth ratio 1:2), 1/3 of the discharge will be placed in the single layer, while 2/3 will be placed in the double layer.

The option *Uniform over depth* is only available for a 3D water quality model.

Type of waste load

Seven types of waste load modelling are supported:

- ◇ Specify flow and concentrations
- ◇ Specify mass
- ◇ Uniform waste load at surface
- ◇ Uniform waste load at bed
- ◇ Uniform waste load at bank
- ◇ Waste load modelling rainfall
- ◇ Waste load modelling seepage en infiltration

The description of these waste loads is followed by the special case of Automated Intake – Outlet coupling.

Specify flow and concentrations

The discharge is specified as a combination of flow rate (in m³/s) and concentration (per m³). If the specified flow is positive, then the values for the substances are used as concentrations and mass is determined by multiplying them with this flow rate. If the specified flow is negative and the concentrations are not zero, the specified concentrations are withdrawn. If the specified flow is negative and the concentrations are zero, the model concentrations will be withdrawn.

Specify mass

The discharge is specified as a load [g/s]. In this case the flow rate is implicitly taken to be one. Withdrawals can be specified using negative loads.

Uniform waste load at surface

The discharge is proportional the surface of the cell, for each computational cell that has a water surface. The general rules for positive/negative flow and (non-)zero concentrations from *Specify flow and concentrations* apply. Specified values are /m².

Uniform waste load at bed

The discharge is proportional to the horizontal surface area for each computational cell that has a water bed underneath. The general rules for positive/negative flow and (non-)zero concentrations from *Specify flow and concentrations* apply. Specified values are /m².

Uniform waste load at bank

The discharge is proportional to the length of a cell's embankment. It is meant to support the effect of diffuse influxes from riparian land into rivers and estuaries. This special waste load requires the presence of a parameter or segment function with the ID `LENGTH` for all cells. To be able to define this parameter in the WAQ-GUI, the following code needs to be add is to the substance file that is used:

```
parameter 'Length'
  description 'Bank length'
  unit        '(m) '
  value       0.0000E-00
end-parameter
```

You need to import the substance file into the WAQ-GUI again after adding the parameter. Specified values are /m.

Waste load modelling rainfall

This is a special case of *Uniform waste load at surface*. The specified concentrations are used by D-WAQ if the flow is positive (rainfall) and zero concentrations are always used if the flow is negative (like for evaporation).

Waste load modelling seepage en infiltration

This is a special case of *Uniform waste load at bed*. This indicates that the specified concentration should be used if the flow is positive (seepage) and that the model concentration should always be used if the flow is negative (for infiltration to the groundwater).

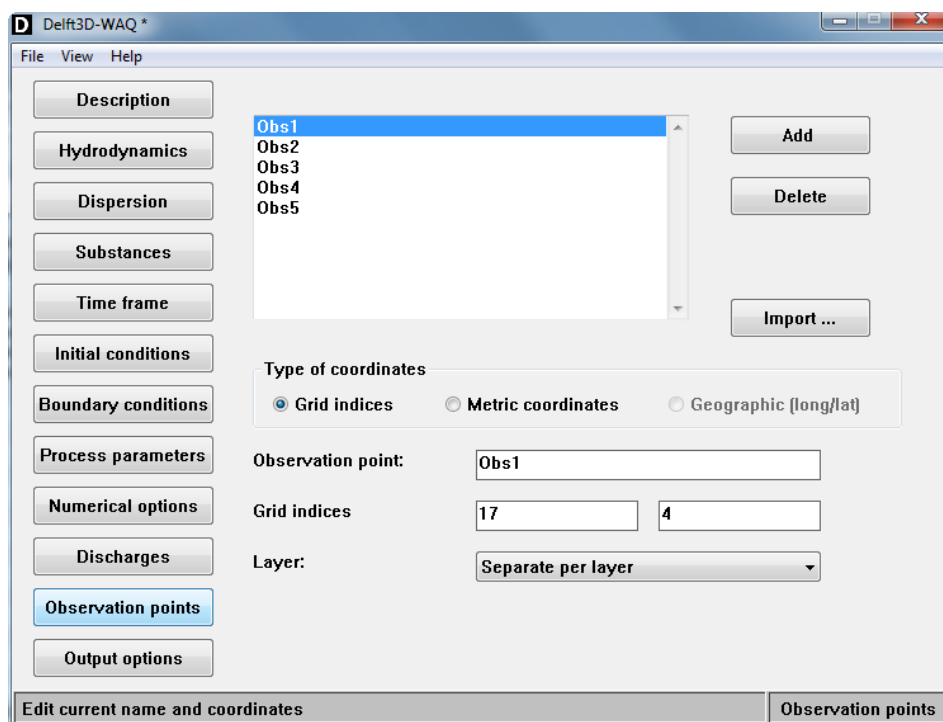


Figure 5.39: Data Group Observation points

Automated Intake – Outlet coupling

When modelling power plants two coupled discharges are used: the water withdrawn at the intake is discharged at the outlet. If the user-defined concentration at the intake is 0 then the concentration at the intake is used in the withdrawn water and the discharged water. If the user-defined concentration at the intake is not 0, then this concentration is used at the outlet. At the outlet the discharge rate and concentration are irrelevant. The mass extracted at the intake is discharged at the outlet.

If the FLOW model contains discharges in the form of power plants, opening the hyd-file will result in couples of discharges with a predefined name: INLETx and OUTLETx, followed by the FLOW discharge name.



Remark:

- ◇ Every time you import a hydrodynamic file <*.hyd> the discharges that are present in the hydrodynamic simulation are added to the list of discharges. The WAQ-GUI does not check if the discharges already exist. If double counting occurs, discharges should be removed from the list.

5.3.11 Observation points

In the Data Group *Observation points* you define the locations (computational cells) for which you want to write information to the history files (<*.his> and <*.hda>), the balance file <*-bal.his> and the monitoring file <*.mon>.

A listing of observation points is shown with three buttons at the right in the upper half of the window. On the lower half the details of the selected observation point are displayed and are available for editing.

There are three ways to specify observation points:

- ◇ Import co-ordinates from an ASCII file
- ◇ Use the **Visualisation Area**
- ◇ Use *Add* and specify co-ordinates in the edit fields

Restriction:

- ◇ The name of an observation point is restricted to 20 characters.



Importing from text file

If you click *Import...*, a dialog appears where you have essentially two choices:

- ◇ Select and use a file with so-called observation areas (file name by default: <*.dmo>). Observation areas are collections of individual computational cells, the concentration in each cell is averaged and the mass balances, if any, are computed for the cells as a whole. There can be only one such file and the contents can not be edited. Instead you can use a program like D-Waq DIDO to generate the file.
- ◇ Select a file with individual cells that become monitoring points (file name by default: <*.obs>).

Files with observation areas are supposed to have the following layout:

```
# Structure of a *.dmo file:
# The file may contain comment lines at the start
# After the comments:
# - The number of observation areas
# - Per observation area:
#   - the name (enclosed in single quotes)
#   - the number of grid cells in the observation areas
#   - a list of indices of grid cells (separated by spaces)
#
# Example:
2
'Area_1' 5
1 2 3 4 5

'Area_2' 4
6 7 8 9
```

Remark:

- ◇ Between the last comment line and the line with the number of areas, there may not be a blank line.



The definition of an <*.obs> file is explained below.

```
# Structure of an *.obs file:
# The file is a comma-separated ASCII-file,
#           containing a header and on each line an observation point.
# The format of the header is fixed!
# The header contains: x-co-ordinate, y-co-ordinate, layer, name
# If layer is 0 then it will be "Uniform over depth".
#
#
# Example:
#   x,      y, layer, name
18000, 22625,    1, central obs-point
13373, 11621,    0, southwestern obs-point
22462, 23552,    4, northwestern obs-point
```

Click *Open* and the observation points are added to the list. Details of each observation point can be adjusted or added if necessary. A warning will be given if an observation point is not within the active model grid.

**Remarks:**

- ◇ The co-ordinates in the <*.obs> file should be in the same projection / co-ordinate system as the model grid
- ◇ Files with observation points should contain the actual grid cell numbers that also take the layer number into account.

Moving Monitoring points

A special feature is the "moving monitoring point" for which the location is not fixed in time. The monitoring point can be used to compare model data with moving measurement devices like drifters or vessels sailing a trajectory. This is a single segment observation point with a name starting with "MOVING", if there exists a function (see process parameters) with exactly the same name then the segment number of the observation point will be set with the value of the function evaluated at the current time. The value of the function is the segment number. Since the value is discrete one should use only block functions to specify a moving monitoring point. If there is no observation for a certain period a value of 0 can be specified. For this period the output of the moving monitoring point will be a missing value. The segment number in the specification of the monitoring point should be given but is not used. To create a list of segment numbers from coordinates is not trivial. Fortran code is available to create the function from coordinates for Delft3D kind of grids.

Example of a function to specify a moving monitoring point called MOVING_Ferrybox:

```
FUNCTIONS MOVING_Ferrybox
BLOCK DATA
2012/01/01-00:00:00      0
2012/01/22-08:24:00     2207
2012/01/22-08:25:00     2206
2012/01/22-08:26:00     2206
...
...
2012/01/22-18:21:00     2091
2012/01/22-18:22:00      0
2013/01/01-00:00:00      0
```

Using the Visualisation Area

Observation points can also be specified with the use of the **Visualisation Area** (menu item *View* → *Visualise area*). After opening, use the *Edit* menu for selecting *Observation points* and use the *Edit Mode* for setting the action (*Add*, *Delete*, *Modify*). If you use *Add*, every

click within the model area will add a new observation point. Details can be specified in the edit fields in the main window. By selecting *Delete* and subsequent clicking on an existing observation point, the point will be deleted. *Modify* means moving the observation point to another location. By selecting this option, you can select an existing observation point, then click a new location within the model grid and the observation point will move to this new location.

Using Add

The third way to add observation points is to use the *Add* button. By clicking *Add*, the list with observation points is extended and is showing "(new)". Specify grid indices or metric co-ordinates (a warning will appear if the co-ordinates are not within the active grid). Other details can be specified as well.

Removing an observation point

Selecting the observation point in the list and clicking *Delete* will delete the observation point (after confirmation).

Layer

The options *Averaged over depth* and *Separate per layer* only apply to a 3D water quality model.

By selecting the option *Separate per layer* for the *Layer* position of the observation point, output will be generated for each layer at that position. In the output files the name of the observation point will be extended with the number of the layer between brackets to distinguish between the layers.

It is useful to specify observation points at locations where data from measuring campaigns are available. Information from observation points may also be used to check input of discharges, or simply the compliance with standards.

5.3.12 Output options

In this data group a selection from the numerous output results can be made in order to reduce the sizes of the output files. Graphical output can be plotted with Delft3D's Graphical Post-Processing package GPP or with QUICKPLOT.

The window is divided into three parts (Figure 5.40), from top to bottom:

- ◇ Timer information
- ◇ File type information
- ◇ Output options (which files, which substances and statistics)

Timer Information

The upper frame (*Times in water quality calculation*) shows the timers specified in the Data Group *Time frame*. They are indicated for informative purposes only, as they are useful to specify the timers for which you would like to have output.

Delft3D-WAQ

File View Help

Description
 Hydrodynamics
 Dispersion
 Substances
 Time frame
 Initial conditions
 Boundary conditions
 Process parameters
 Numerical options
 Discharges
 Observation points
 Output options

Times in water quality calculation

Start time: 05 08 1990 12 30 00
 Stop time: 15 08 1990 12 30 00
 Time step: 00 00 0000 00 15 00
 Reference time: 05 08 1990 00 00 00

| Type | Start time dd mm yyyy hh mm ss | Stop time dd mm yyyy hh mm ss | Time interval dd mm yyyy hh mm ss |
|---------|-----------------------------------|----------------------------------|--------------------------------------|
| Monitor | 05 08 1990 12 30 00 | 15 08 1990 12 30 00 | 00 00 0000 06 00 00 |
| History | 05 08 1990 12 30 00 | 15 08 1990 12 30 00 | 00 00 0000 01 00 00 |
| Map | 05 08 1990 12 30 00 | 15 08 1990 12 30 00 | 00 00 0000 02 00 00 |

Options

Files Output files? Statistics
 Select Parameters to output? Balances

Output options

Figure 5.40: Data Group Output options

Output timers

D-WAQ generates three main types of output files:

1. Monitor output
Results for observation points will be printed in an ASCII report file <*.mon>. Results will be given in the period with a start time, a stop time and a certain time interval. *Start time*, *Stop time* and *Time interval* for this output can be specified in the corresponding edit fields. Default: time interval in coupled hydrodynamics.
2. History output
Time-series information for the observation points will be written to either a binary file or a NEFIS file (or both). *Start time*, *Stop time* and *Time interval* for this output can be specified in the corresponding edit fields. Default: time interval in coupled hydrodynamics.
3. Map output
Spatial plots of concentration distribution will be written to either a binary file or a NEFIS file (or both). *Start time*, *Stop time* and *Time interval* for this output can be specified in the corresponding edit fields. Default: time interval in coupled hydrodynamics.

Output files

By pressing *Files* you can specify the *Type of output files* in the **Select output files** window (Figure 5.41).

D-WAQ produces output files suitable for several platforms: output files can be either:

- ◇ PC based (binary or NEFIS) or:
- ◇ Linux/UNIX based (binary/unformatted or NEFIS);

NEFIS and binary files contain the same information, so that it is not necessary to select both (if you select both, a lot of redundant information is stored).

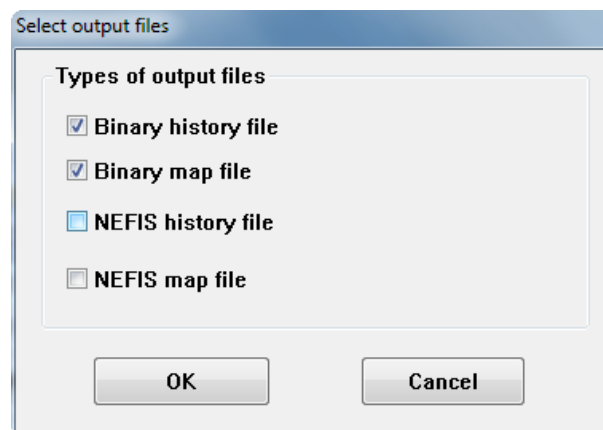


Figure 5.41: Specification of output files. The output in NEFIS format is switched off

For post-processing using GPP or QUICKPLOT you need to specify the following data set/file types.

- ◇ binary/binary-unformatted;
 - DELWAQ | binary history file (<*.his>);
 - DELWAQ | binary map file (<*.map>);
- ◇ NEFIS:
 - DELFT3D | water quality history file (<*.hda>);
 - DELFT3D | water quality map file (<*.ada>);

Parameters to output

You can (un)select specific output parameters for the different types of output files. Press *Select* at the bottom of your window; the **Select output to files** window will pop up.

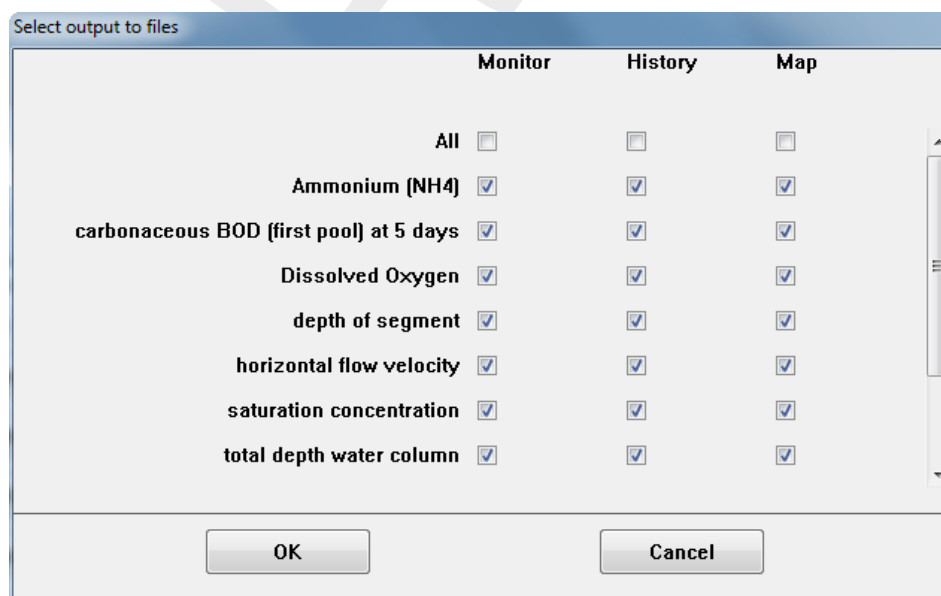


Figure 5.42: Select output to files window

You may activate the kind of output required by ticking on or off the check box. You can use the checkbox *All* to (un)select the whole column for that output file at once.

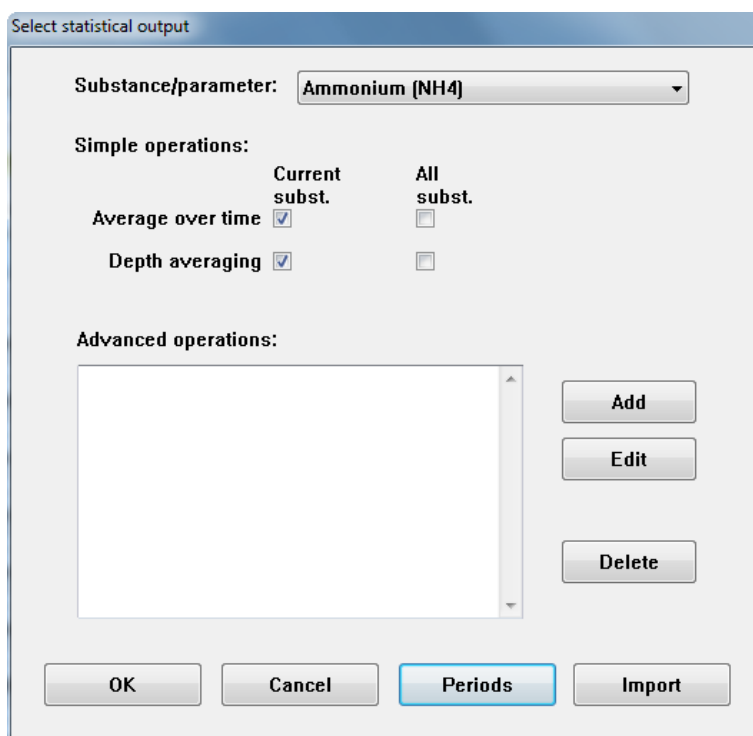


Figure 5.43: Select statistical output main window

Statistics

By clicking *Statistics*, you can specify statistical output of your water quality calculation. The **Select statistics output** window is displayed in [Figure 5.43](#).

For more information on the statistical output functions see [Appendix C](#).

The window consist of a drop-down list containing all substances and checkboxes to switch statistics on or off. Checkboxes for every substances and output parameter are available. You can use *All subst.* to switch all substances on/off. Statistics are divided into:

- ◇ Average over time
- ◇ Depth averaging
- ◇ Advanced operations

The selected statistics are generated for each defined period.

At the bottom, the following options are available:

- ◇ *OK* - Confirming your statistical output settings and go back to the main **Output options** window.
- ◇ *Cancel* - Cancelling your statistical output settings and go back to the main **Output options** window.
- ◇ *Periods* - Specification of the time periods to use in the statistical analysis.
- ◇ *Import* - Select and import an existing statistical file <*.stt>.

Defining Periods

In order to retrieve statistical output, you can define specific period(s) for which you want to have statistical output. By clicking *Periods* you can specify new periods or get an overview

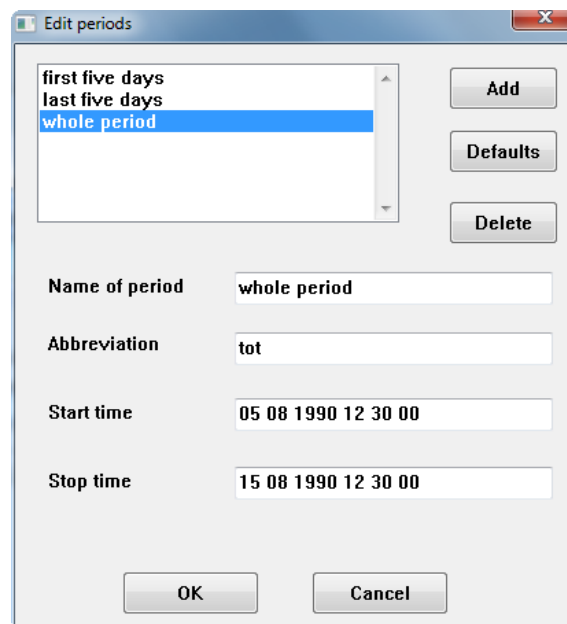


Figure 5.44: Periods in statistical output

of the periods you have defined so far (Figure 5.44). A period is defined by its name, a start time and a stop time. An abbreviation is used to distinguish the periodical statistical output in the output files (<*.map>, <*.his>, <*.mon>, etc.). Statistical output is generated for each period. For example, in Figure 5.44 three periods are defined. If *Average over time* is selected, an average value will be calculated for the three periods independently. Note that periods may overlap.

The *Add* button adds a period to the list. You can specify name, abbreviation, start and stop time in the edit fields underneath the list. *Delete* will remove the selected period. By clicking *Defaults*, the start and stop time of the selected period will be set to the start and stop time of the water quality calculation as specified in the Data Group *Time frame*.

Output files

Two additional files are generated that contain the output of the statistical analysis:

- ◇ A monitor file containing the monitor output (<*-stat.mon>). This is an ASCII file containing the values for all observation points defined in the Data Group *Observation points*.
- ◇ Map file (<*-stat.map>) containing the statistical output for every grid cell of the model area.

Statistical time-series such as daily averages are added to the history file (<*.his> or <*.hda>).

Average over time (Standard Statistics)

For the standard statistics the following output is produced per period:

- ◇ Minimum value
- ◇ Maximum value
- ◇ Mean value
- ◇ Standard Deviation

Depth averaging

For the depth averaging statistics the following output is produced per period:

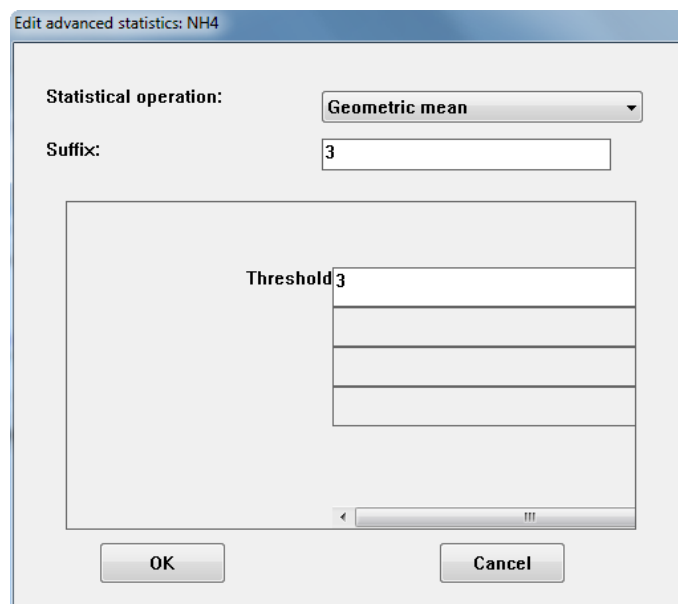


Figure 5.45: Advanced statistics window. For NH4 three advanced statistics are defined: periodic averages, exceedance times, and a 90% quantile

- ◇ Minimum depth average value
- ◇ Maximum depth average value
- ◇ Mean depth average value
- ◇ Standard deviation of the depth average value

Advanced statistics

By clicking *Add* or select an advanced statistical operation and then *Edit*, the **Edit advanced statistics** window will open (Figure 5.45).

Four advanced operations are available:

- ◇ *Geometric mean*: Useful for substances with a large range and relatively high values (e.g. coliform bacteria concentrations). You have to set a *Threshold* value as well, as negative and zero values are not allowed in a geometric (i.e. logarithmic) mean calculation.
- ◇ *Periodic averages*: If you want to have for example hourly or daily averages, you can use the data-time string ("dd mm yyyy hh mm ss") to set this *Period*. Daily averages will be "01 00 0000 00 00 00"). You can specify a *Start time*, if necessary.
- ◇ *Percentage (Exceedance time)*: This statistical method calculates the time that the selected substance is above (*Exceedance* = "Yes") or beneath (*Exceedance* = "No") a certain value (*Critical concentration*). You have to specify the critical value.
- ◇ *Quantiles*: This method calculates the value that is not being exceeded for a certain % of the time (*Quantile in % to be reported*). You can specify the *number of buckets* (more bins is more accurate) and a *lower and upper boundary*. The actual concentration that you model, should fall within this range.

By using *Add* you can add a statistical operation. By clicking *Edit* you can redesign and by clicking *Delete* you can delete the advanced statistics for the selected substance or output parameter.

If you switch to another data group (after closing all relevant windows of the statistics) the statistical specifications will be stored in a separate file, the <*.stt> file. You can re-use this

file in other water quality calculations by using the *Import ...* option in the **Select statistical output** window (Figure 5.43).

Balances

The balance output for D-WAQ includes a number of options (see Figure 5.46)

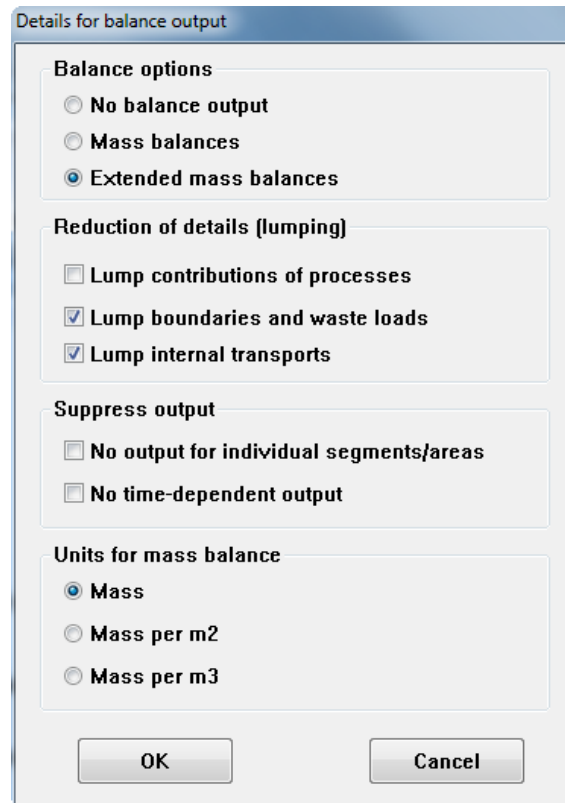


Figure 5.46: Details for balance output window

- ◇ The overall option selects the type of balance information:
 - *No balance output*: there will be no information about mass balances beyond what is written to the monitoring file.
 - *Mass balances*: The computational program will write detailed information about the mass balances (transport fluxes of each substance, contributions of the various water quality processes and so on) in the monitoring points and monitoring areas to a separate history file.
 - *Extended mass balances*: The program will write extra information with respect to the model area as a whole to a report file.
- ◇ A number of sub-options are available with the extended mass balances option:
 - The level of detail can be set:
 - You can either have the contribution of all individual processes reported or have them “lumped” into a single term.
 - The same thing is separately possible with transports over the boundaries and waste loads and with the internal transports.
 - You can suppress output for individual monitoring points (segments) and monitoring areas (leaving only the overall mass balance term) and for the monitoring timesteps (leaving only the terms accumulated over time).

These options are meant to help you get a useful report:

- If you want an overview, then suppressing a lot of the details can help you to focus on the overall features.
- However, if you have a problem (some strange or unexplained results in some region of the model for instance), then it can be very helpful to get as much details as you can.
- In general, the overall report gives you insight in the behaviour of the model as a whole.
- ◇ The unit for the mass balance terms can be selected:
 - The terms can simply be the total mass [g].
 - The terms can be divided by the total surface area [g/m²].
 - The terms can be divided by the total volume [g/m³].

Each option can be useful at times, depending on the kind of analysis you want to make.

5.3.13 Saving the scenario file

As you went to all data groups, the input for the scenario is now completed. Under the menu item *File*, you can *Save* (or *Save As...*) the scenario. Note that the extension of the scenario should be *<*.scn>*. This file stores the scenario for further adaptation or inspection with the WAQ-GUI. Simultaneously, a file with the extension *<*.inp>* is saved with the same run ID as the *<*.scn>* file. The *<*.inp>* file is used by the pre-processors and the water quality module.



Restriction:

- ◇ The run ID may not contain blanks.

5.3.14 Addition of a sediment grid

After completion of the model set-up (substances, processes, hydrodynamics, computational grid, loads, forcing, boundaries, etc.) a sediment grid can be added to the water grid. However, this is not supported by the present GUI. Once you have produced a complete model input file and ran the resulting model successfully using the WAQ-GUI, the sediment grid and the additional required input with respect to the sediment (composition, transport process, deep boundary, etc.) can be added to the input file (ascii) by means of manual editing. Two additional user manuals are available for this: 'Documentation of the input file' and 'Sediment Water Interaction'.

6 Running and post-processing (Delft3D)

6.1 Running

6.1.1 Pre-processing: input verification

After definition of a water quality scenario the simulation can be carried out. Basically, running a simulation involves three steps:

- | | |
|-------------------|---|
| 1 Pre-processing | Check whether the input for the simulation is complete and correct. |
| 2 Processing | Carry out the simulation and generate output. |
| 3 Post-processing | Check the output and present results. |

Pre-processing a water quality simulation is easy. By clicking *Waq (1)* in the **Water quality and ecology** window, the pre-processing is started.

By clicking *Waq (1)* a file selection window is opened (Figure 6.1) in which you have to specify the name of the input file <*.inp>. The input file <*.inp> has the same run ID as the scenario file <*.scn>; they are both saved by the WAQ-GUI. A file can be selected through the *Select file* dialogue. However, it is required that the input file <*.inp> is located in the working directory. If this is not the case, you will have to change the working directory first. How to change the working directory is described in [section 4.3](#).

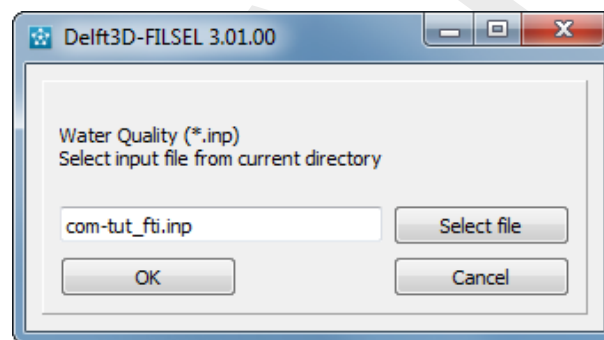


Figure 6.1: Select input file

The pre-processor runs in a new window, see [Figure 6.2](#).

You can close this window if the pre-processor finishes with a 'Normal end'.

The pre-processing generates two files that are available for inspection:

- 1 List file <*.lst>
The list file <*.lst> checks whether the input is complete and the syntax of the input file <*.inp> is correct.
- 2 Report file <*.lsp>
The Report file <*.lsp> (or 'list of processes' file) determines which water quality processes are selected (switched on) and determines where to retrieve the parameter input for the processes.

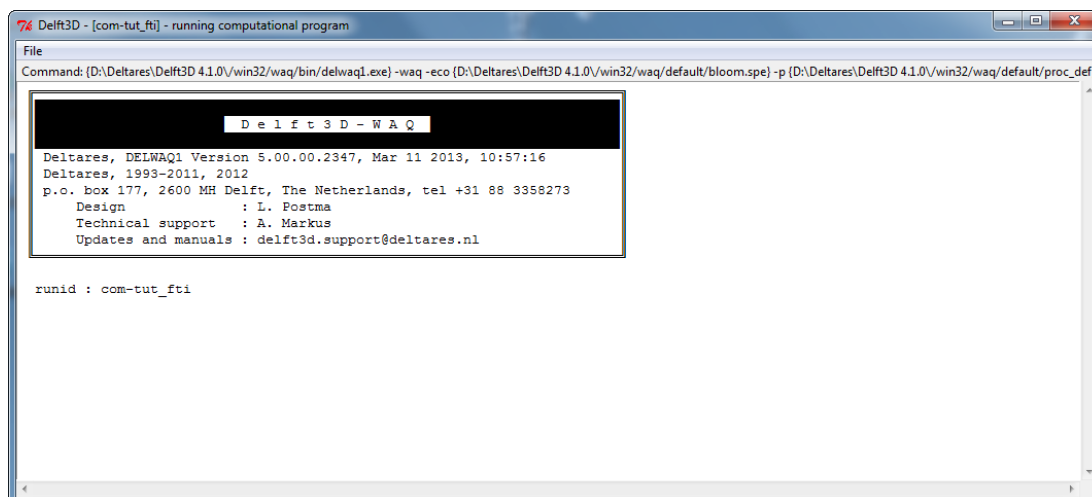


Figure 6.2: Window with running information about the WAQ pre-processor

6.1.2 List file <*.lst>

The list file <*.lst> can be reviewed through the *Reports | Input* options in the **Water quality (WAQ)** selection window (Figure 4.3). The file will be opened in the default text editor. The list file <*.lst> is in ASCII format and can be inspected in every text editor.

The list file <*.lst> provides an overview of all the input specified in the WAQ-GUI. Usually it is no use trying to review the complete file. One of the last lines of the list file <*.lst> should read:

```
Number of ERRORS during input : 0
```

If errors are found, you can search for the word 'ERROR' in the <*.lst> to find the place of the error. Subsequently, changes can be made in the WAQ-GUI. If the input file <*.inp> was generated with the WAQ-GUI, errors are normally not encountered.

Apart from errors, the list file <*.lst> may give warnings. As the number of warnings is not given at the end of the list file <*.lst>, you should always look for the word 'WARNING' in the list file <*.lst>. Warnings usually deal with non-existing files, for example when files are moved to another directory.

6.1.3 Report file <*.lsp>

The report file <*.lsp> can be reviewed through the *Reports | Processes* options in the **Water quality (WAQ)** selection window (Figure 4.3). The file will be opened in the default text editor. The reports file <*.lsp> is in ASCII format and can be inspected in every text editor.

The report file contains the blocks listed below. The blocks are separated by the '#' character.

- #1 Overview of processes that are switched on and determination per process whether the input is complete. A warning is given if the input is incomplete.
- #2 Fluxes, velocities and dispersions per substance.
- #3 Additional processes for process-output only.
- #4 Detailed process-input items for each active process.
- #5 Identification if input parameters defined by you that are not used by the process system.
- #6 Locating requested output from active processes.

- #7 Updated memory requirement for the computational core (delwaq2).
- #8 Presented messages (information, warning and errors).

Block 1

An overview of all processes selected in the substance file <*.sub> and thus all processes that are included in the water quality simulation. For each active process is reported if the input is complete. If this is the case, the report file <*.lsp> contains the following message:

```
Input for [RearOXY  ] Reaeration of oxygen
Process is activated
```

Such a message is given for every activated process.

If for one or more input parameter no input is available a warning is given. The parameter for which no input is available is specified like in the following message:

```
Input for [RearOXY  ] Reaeration of oxygen
WARNING : activated process can NOT be switched on
Not found:[Depth    ] depth of segment
```

Usually, the parameter has a missing value which can be specified either by entering a value or deriving it from another process. You should go back to the WAQ-GUI or the PLCT to resolve the problem. Note that the water quality simulation will run anyway: only the processes are not taken into account resulting in an unwanted and therefore incorrect result. It is therefore important that you check if all the processes are activated correctly.

Block 2

This is a very important block for you to check whether the right selection of processes from the library has been made.

In this block an overview of the activated fluxes, dispersions and velocities that act on each selected substance is given. Furthermore, you are informed which process will calculate the flux, dispersion or velocity. So, except for the advective transport fluxes and discharges, this block gives you the terms of the mass balance for each substance.

In the example below, four fluxes, one dispersion and no (settling) velocities for dissolved oxygen (OXY) are found in the library (fictive example). The dispersion and the four fluxes are used in the simulation; no velocities are found.

```
-Fluxes for [OXY      ]
Found flux [dNITRIF   ] nitrification flux
from proces [Nitrif\_NH4] Nitrification of ammonium
Process is switched on.
Found flux [dREAROXY  ] reaeration flux
from proces [RearOXY  ] Reaeration of oxygen
Switching [RearOXY  ] on.
Found flux [dOxyBODCOD] oxygen consumption flux of BOD and COD
from proces [BODCOD   ] Mineralisation BOD and COD
Process is switched on.
Found flux [dOxSOD    ] oxygen consumption from SOD
from proces [SedOXYDem] Sediment oxygen demand
Switching [SedOXYDem] on.
-Dispersion for [OXY      ]
Found dispersion[VertDisp ] vertical dispersion
from proces [VertDisp  ] Vertical dispersion (segment -} exchange)
Process is switched on.
```

```
-Velocity for [OXY      ]  
No velocity found
```

Block 3

This block lists the additional processes that are switched on as a result of the segment related process-output requested by you. The first item between straight brackets is the name of the process (e.g. [DynDepth]) that calculates the requested output which is specified in the second item between straight brackets (e.g. [Depth]).

```
# Locating processes for requested output  
Switching [DynDepth  ] on for output [Depth      ]  
Switching [Veloc     ] on for output [Velocity   ]  
Switching [SaturOXY  ] on for output [SaturOXY   ]  
Switching [TotDepth  ] on for output [TotalDepth]
```

Block 4

In this block the status of all the processes that are switched on and for which the input is complete is reported to you. For each process the report file <*.lsp> specifies what information is used for each parameter.

Information can be retrieved in eight different ways:

- 1 substance: The process parameter is included as a substance.
- 2 output from process: The process parameter is derived from another process.
- 3 segment function: The process parameter is included as a segment function (variable in both time and space).
- 4 function: The process parameter is defined as a time-series (variable in time only).
- 5 parameter: The process parameter is included as a parameter (variable in space only).
- 6 DELWAQ: The process parameter is derived from the hydrodynamic model or an internal D-WAQ variable for which no further specification is necessary.
- 7 constant: You have specified a constant value for the process parameter in the WAQ-GUI <*.scn>.
- 8 default: No input is specified in the WAQ-GUI <*.scn>, the default value is used. The default value is given as well.

Except for the 'parameter' all types of input occur in the example below:

```
Input for [RearOXY  ] Reaeration of oxygen  
[OXY      ] Oxygen  
Using substance nr 3  
[Depth    ] depth of segment  
Using output from proces [DynDepth  ]  
[Temp     ] ambient water temperature  
Using function nr 1  
[Velocity ] horizontal stream velocity  
Using output from proces [Veloc     ]  
[VWind    ] wind velocity  
Using constant nr 5  
[SWRear   ] switch for oxygen reaeration formulation \file{1-11}  
Using constant nr 6  
[KLRear   ] reaeration transfer coefficient  
Using constant nr 7  
[TCRear   ] reaeration temperature coefficient  
Using default value: 1.01600  
[DELT     ] timestep for processes  
Using DELWAQ timestep in days  
[SaturOXY ] saturation concentration
```

```

Using output from proces [SaturOXY ]
[Salinity ] Salinity
Using segment function nr 1

```

The numbers for the respective constants and (segment) functions refer to the order in the scenario file <*.scn> (or the input file <*.inp>). For the values refer to these values or check in the WAQ-GUI.

Block 5

In this block the input that is not recognised by the process system, is listed. Always check block 5 of the report file! If an item is incorrectly spelled and not recognised by the process system probably a default is used. Check the correct spelling either in block 4 of the report file or in the Technical Reference Manual.

```

# Determine the use of the DELWAQ input
Constant [RcDetQ          ] is NOT used by the process system
Parameter [Depht          ] is NOT used by the process system
Function [Tempp           ] is NOT used by the process system
Segment function [Zurfp    ] is NOT used by the process system

```

Block 6

The sixth block of the report file <*.lsp> specifies the origin of all output parameters you request. Output variables are included in the substance file <*.sub> and can be reviewed in the WAQ-GUI. Output variables can be derived from processes as shown in the example below, but can also be constants, default values, (segment) functions or parameters. Note that the substances themselves are not reported here. They are by default included in the output.

```

# Locating requested output from active processes
Output [Depth      ] from proces [DynDepth ]
Output [Velocity   ] from proces [Veloc   ]
Output [SaturOXY   ] from proces [SaturOXY ]
Output [RCREAR     ] from proces [RearOXY  ]
Output [SatPercOXY] from proces [RearOXY  ]
Output [TotalDepth] from proces [TotDepth ]
Output [LocalDepth] from proces [TotDepth ]

```

Block 7

This block gives some technical information on computer memory etc. The information is only in rare exceptions relevant for water quality simulations and can be taken for granted.

Block 8

Finally, the last block indicates the number of informative messages, warnings and errors. All messages should be checked, as they may or may not be of relevance to you.

6.1.4 Running D-Water Quality

After pre-processing and checking that the input is correct, you can run the water quality simulation. Click *Waq (2)* to start the simulation. No input file is requested anymore as it is assumed that the last pre-processed input file (in the current working directory!) is the one to be run. Make sure that you pre-process first after you made adaptations, before running a simulation, otherwise these adaptations will not be incorporated in the actual simulation. The pre-processors generate a ranges of temporary working files <*.wrk> that are used in

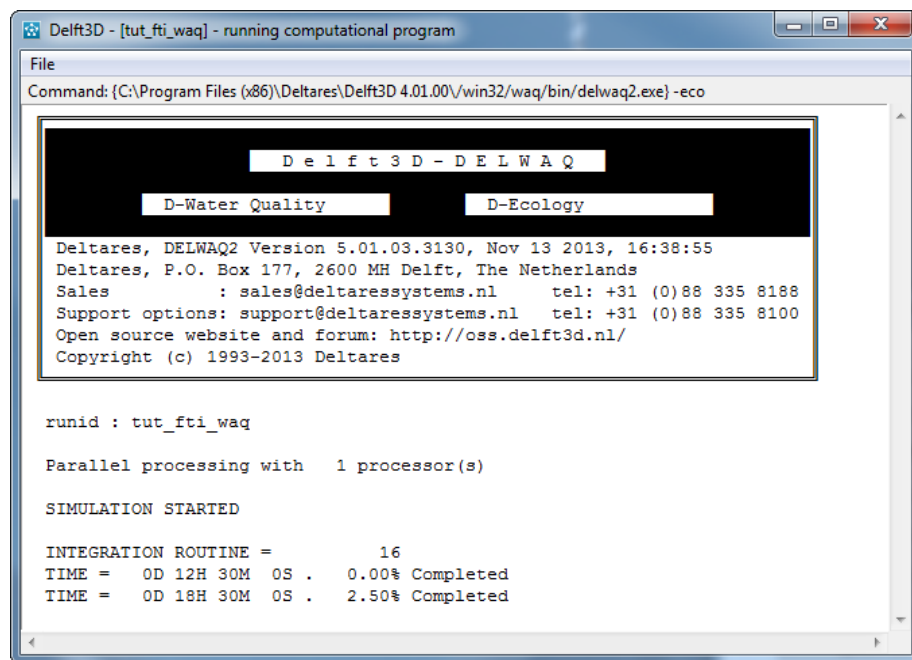


Figure 6.3: Running a simulation. The simulation time relative to the reference time is displayed

Table 6.1: Output files of D-WAQ and post-processing program

| type of output | file type | file extension (format) | post-processing program |
|----------------|--------------|-------------------------|-------------------------|
| time-series | history file | <*.his> (binary) | GPP, QUICKPLOT |
| spatial | map file | <*.hda> (NEFIS) | GPP, QUICKPLOT |
| mass balance | balance file | <*.map> (binary) | GPP, QUICKPLOT |
| monitor | monitor file | <*.ada> (NEFIS) | GPP, QUICKPLOT |
| | | <*-bal.his> (binary) | GPP, QUICKPLOT |
| | | <*=bal.prn> (ASCII) | text editor |
| | | <*.mon> (ASCII) | text editor |

the water quality simulation. If you do not run the pre-processors, *Waq* (2) will use the old <*.wrk> files.

The simulation runs in a new window. The progress of the simulation can be viewed relative to the reference time of the simulation (Figure 6.3). The time step is determined by the time step of the monitoring file; refer to [section 5.3.12](#) on how to change this time step.

6.2 Post-processing

6.2.1 Output files

A D-WAQ simulation generates different types of results ([Table 6.1](#)).

Time-series and spatial information are available in two formats: binary and NEFIS. As they contain exactly the same information, usually only one type of format is selected. The type of format can be selected in the *Output options* Data Group (refer to [section 5.3.12](#)). Time-series information is saved for every observation point specified. Spatial information is saved for all computational elements. Refer to the GPP and Delft3D-QUICKPLOT User Manuals on how to visualise the results ([GPP UM, 2013](#); [QUICKPLOT UM, 2013](#)).

Mass balances are available if the balance output option is selected in the *Output options* Data Group. Mass balance information is available for every substance for every observation point specified. The balance terms represent the accumulated fluxes during the time step in the monitor file. For example, if the time step in the balance file is one day, the unit of the fluxes is g/d. If the time step in the balance file is one week, the unit of the fluxes is g/week. The balance file <*-bal.his> has the same time step as the monitor file <*.mon>. Refer to the GPP User Manual on how to visualise the results.

The monitor file <*.mon> contains information per observation point such as concentrations of the substances and values of the output parameters. Also, a total mass balance for the complete model area is given consisting of the terms: total mass in system, changes by processes, changes by loads, boundary inflows and boundary outflows. The balance terms represent the accumulated fluxes during the time step in the monitor file.

If the balance output option is switched on, a mass balance consisting of the same terms is included for each observation point in the monitor file <*.mon>. Note that contrary to the balance file <*-bal.his> no individual process fluxes are specified in the monitor file <*.mon>.

DRAFT

7 Tutorials

This tutorial contains two sections, one section about the 2/3-dimensional Delft3D-suite for free surface flows, see [section 7.1](#), and one section about the 1/2-dimensional SOBEK-suite for free surface (1D/2D) and pressurized (1D) flow, see [section 7.2](#).

7.1 Tutorial D-Water Quality for free surface flow (Delft3D-WAQ)

7.1.1 Introduction

This chapter can be used to get acquainted with the procedure to set up a water quality calculation. A schematised case is used to guide you through the different steps and actions necessary to perform a simulation.

The tutorial case concerns the area of the 'Friesian Tidal Inlet', which represents an opening between the islands Ameland and Schiermonnikoog. We will perform a simulation of E.Coli bacteria on a $1 \times 1 \times 2$ aggregation of the hydrodynamic database.

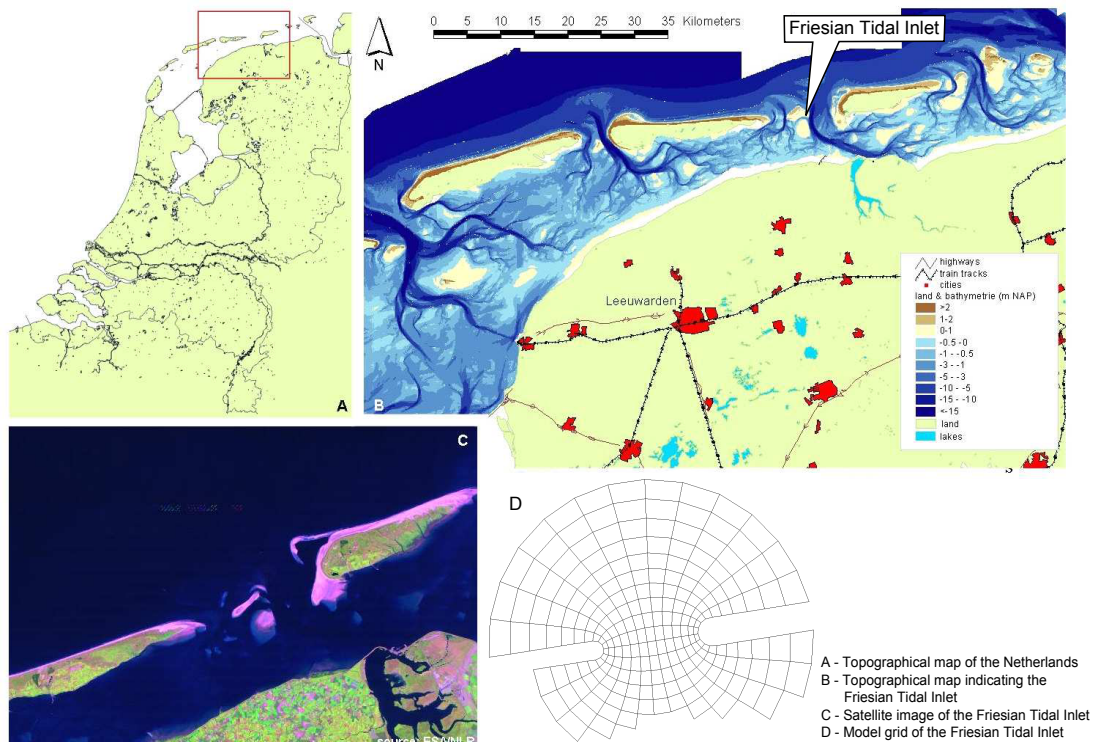


Figure 7.1: 'Friesian Tidal Inlet': an opening between two islands in the north of The Netherlands

This chapter gives both *descriptive* information about the steps to take to set up a water quality calculation and *GUI-operations* to complete each step. The *GUI-operations* are displayed in the textboxes with the grey header.

The input data will be generated on the directory <.../tutorial/waq/friesian_tidal_inlet>

7.1.2 Specifications of tutorial case 'tut_fti_waq'

Table 7.1 presents the specifications of the tutorial case.

Table 7.1: Specifications of tutorial case 'tut_fti_waq'

| | |
|----------------------------|--|
| Area | Friesian Tidal Inlet |
| Hydrodynamic database | 12.5 hours, 15 min time step (<com-tut_fti_waq.dat>, <com-tut_fti_waq.def>) |
| Horizontal aggregation | inactive cells removed |
| Vertical layer aggregation | 5 water quality layers (10 hydrodynamic layers) |
| Time step aggregation | none |
| Substance | E.Coli |

The D-WAQ model framework is started from the Delft3D-MENU as described in Chapter 5.

1. STARTING THE DELFT3D-MENU

Start Delft3D

- ◇ Start Delft3D-MENU by using the desktop icon/Start button.
- ◇ Click *Water Quality*.
- ◇ Click *Select working directory*, and browse to the tutorial directory:
<.../tutorial/waq/friesian_tidal_inlet>
- ◇ Click *OK* to confirm and to close the selection of your current working directory.

7.1.3 Conversion of the hydrodynamic results

7.1.3.1 Coupling module

2. STARTING THE COUPLING MODULE

- ◇ In the **Water quality and ecology** window, select *Coupling* (Figure 4.3).
- ◇ To start the COUP-GUI, select *Define input*, see Figure 5.8.

You are now accessing the GUI of the coupling module (Figure 5.10). The GUI is similar to the general WAQ-GUI, but only the first three data groups are enabled. They will be described in the following section.

7.1.3.2 Definition of the input

The three datagroups which are enabled are:

- ◇ Description
- ◇ Hydrodynamics
- ◇ Dispersion

The menu-items *File* and *Help* are also available.

7.1.3.2.1 Description

With *Description* you can add a file description in order to produce some meta-information about the coupling. Three lines of descriptive information are available.

| 3. EDITING THE DESCRIPTION DATA GROUP |
|--|
| <ul style="list-style-type: none"> ◇ In the COUP-GUI, click <i>Description</i>. ◇ Enter 3 lines (of max. 39 characters) of meta-information. <ol style="list-style-type: none"> 1 Friesian Tidal Inlet 2 Hydro: Flow tutorial with 10 layers 3 WAQ: Vertical aggregation to 5 layers ◇ See Figure 5.10. |

7.1.3.2.2 Hydrodynamics

With the Data Group *Hydrodynamics* the hydrodynamic database is selected. By clicking *Com-file*, you can browse to and select one single <com-name.dat> file, which can be found in the <delft3d\tutorial\waq\friesian_tidal_inlet\input_waq_fti> directory. By clicking *Open*, the <com-tut_fti_waq.dat> file will be loaded into the GUI and information about this file will be displayed.

Aggregation in time

The timers in the file will automatically appear in the *Time information* frame. Time steps can be increased, for example in order to reduce the required disk space for storage. Hereto, adapt the time step in the menu, but increase it only with an integer number (2 times, 3 times etc.).

In this tutorial we do not aggregate in time, so no adjustment of timers is needed.

Horizontal aggregation

The grid can be aggregated in the horizontal within the frame *Horizontal aggregation*. Select under *Type of* either:

- ◇ *No aggregation*: no spatial aggregation is used.
- ◇ *Use aggregation file (DIDO)*: This option requires an administration file (<*.dwq>) and can be either created or selected by you. A <*.dwq> file is created by the grid editor DIDO. This WAQ tool can be activated from Delft3D-MENU. Consult the DIDO User Manual for details about the spatial aggregation.
- ◇ *Remove inactive cells*: all dry segments are deleted automatically.

In this tutorial the option of *Remove inactive cells* is chosen (see [Figure 7.3](#)).

Vertical aggregation

Layers can be aggregated in the vertical using the layer editor under button *Edit layers*. This tutorial case contains 10 (hydrodynamic) layers. If no vertical aggregation is chosen, the number of water quality layers is equal to the number of hydrodynamic layers. To reduce storage space and decrease calculation time, the number of water quality layers can be reduced. Select *Edit layers*. [Figure 7.2](#) will appear.

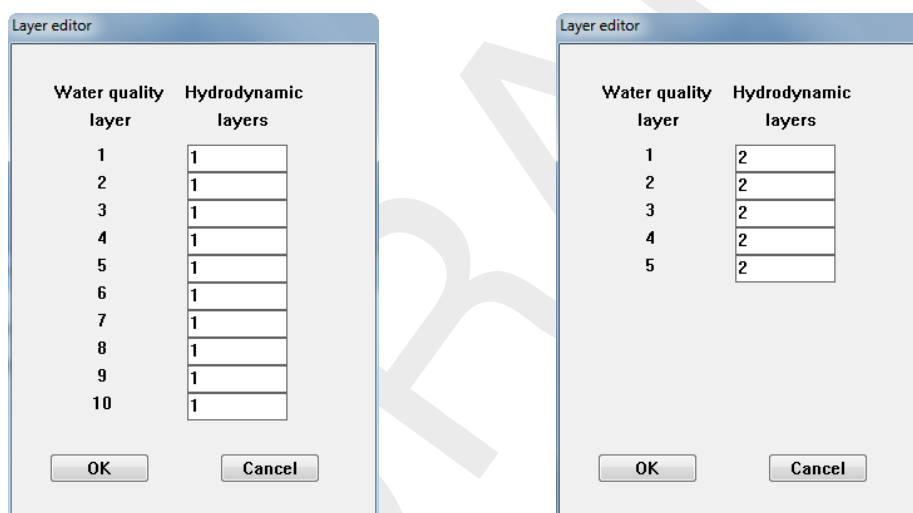


Figure 7.2: Vertical aggregation using the Layer editor

On the left part of the **Layer editor** window, the number of water quality layers is shown. On the right-hand side, the corresponding number of hydrodynamic layers is shown. By changing the number in the input boxes (more than one hydrodynamic layer are combined to one water quality layer), the number of water quality layers decreases.

- ◇ Create 5 water quality layers by, starting from the top, change the number of hydrodynamic layers from 1 to 2, see [Figure 7.2](#).



Remark:

- ◇ The number of hydrodynamic layers remains intact ($2 + 2 + 2 + 2 + 2 = 10$). Many other aggregations are possible: for example $2 - 3 - 3 - 2$ (i.e. 4 water quality layers and $2 + 3 + 3 + 2 = 10$) or $3 - 4 - 3$ (i.e. 3 water quality layers and $3 + 4 + 3 = 10$).

4. SPECIFYING AND AGGREGATION THE HYDRODYNAMIC DATABASE

- ◇ In the COUP-GUI, click *Hydrodynamics*.
- ◇ Click *Com-file*, and browse to the <.../tutorial/waq/friesian_tidal_inlet> directory to select the <com-tut_fti_waq.dat> file.
- ◇ Click *Open* to confirm (note that the details will be displayed in the *Time information* frame).
- ◇ In the *Horizontal and vertical aggregation* frame, select *Remove inactive cells* from the *Type of* drop-down box.
- ◇ In the *Horizontal and vertical aggregation* frame, click *Edit layers*.
- ◇ From top to bottom, change in the first 5 entry boxes the “1” into “2”.
- ◇ Click *OK* to confirm.
- ◇ See Figure 7.3.

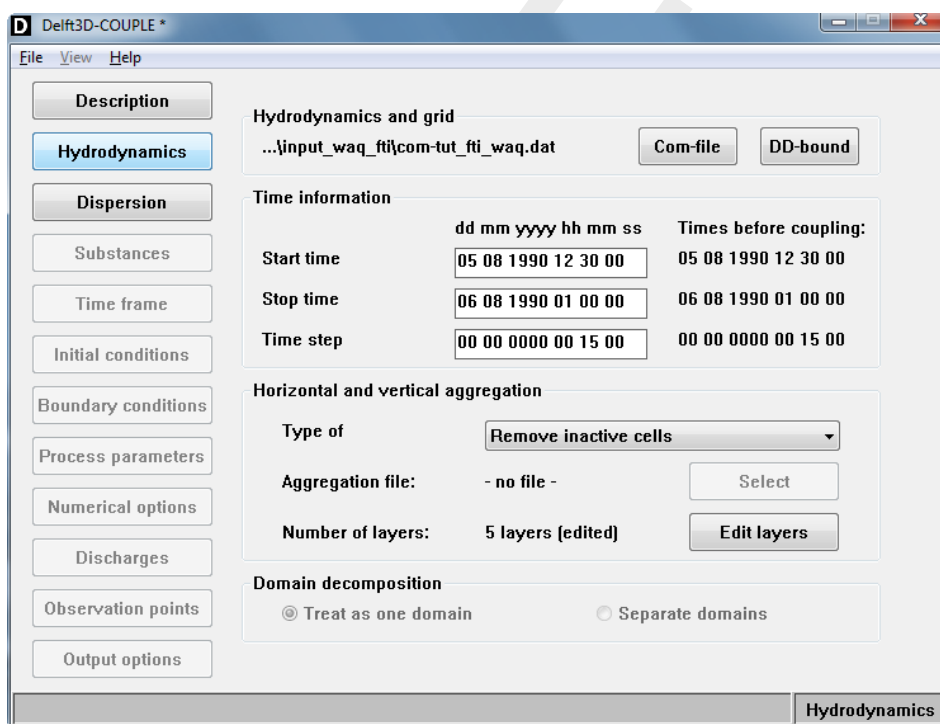


Figure 7.3: COUP-GUI - Data Group Hydrodynamics

7.1.3.2.3 Dispersion

Within the Data Group *Dispersion* you can choose to use the vertical diffusion from the hydrodynamic simulation. You can specify an interface depth and diffusion coefficients above and below this interface.

In this tutorial case, the minimum vertical diffusion from the hydrodynamics is not used.

5. EDITING DISPERSION

- ◇ In the COUP-GUI, click *Dispersion*.
- ◇ Inspect and do not change the (default) values.

7.1.3.3 Saving input and running the coupling module

By selecting *File* → *Save (As)* you are requested to save the file. Your *current working directory* is the right location. Give the filename <com-tut_fti_waq.hyd>. The extension <hyd> will be given automatically on Windows platforms. Exit the GUI by selecting *File* → *Exit* from the menubar, returning to the **Hydrodynamic coupling** window. Select *Start* and the coupling module will start. A window will be opened in which the coupling of the hydrodynamical database is carried out (see Figure 7.4). When the window displays 'Conversion has been done', you can close this window.

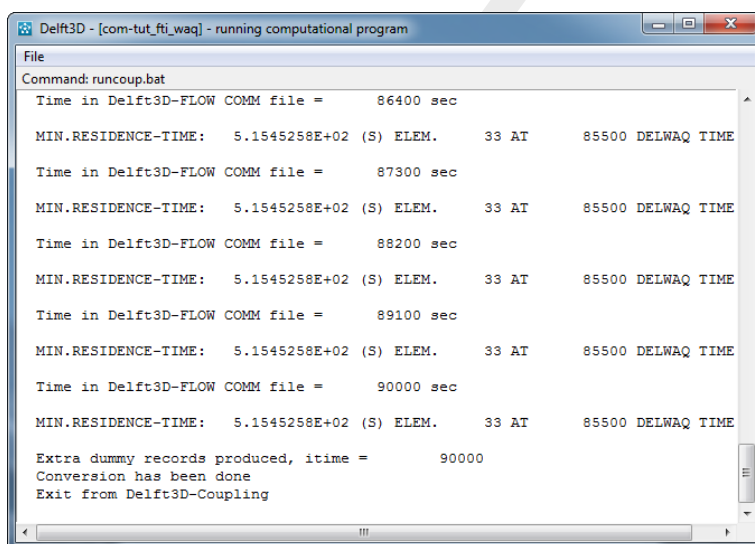


Figure 7.4: Screen output of the Coupling program

Result files of the coupling will be available in your *current working directory*. An interesting file to inspect is the <couplnef.out>.

6. SAVING INPUT AND RUNNING THE COUPLING

- ◇ In the COUP-GUI, select *File* → *Save As...* and save the file as <tut_fti_waq.hyd> in your current working directory.
- ◇ Exit the COUP-GUI by selecting *File* → *Exit*
- ◇ Click *Start*, select the file <tut_fti_waq.hyd> and after pressing *OK* the coupling will start in a new window.
- ◇ As soon as 'Conversion has been done' is displayed, close the window.
- ◇ To inspect the results, first go back pressing the button *Return*, next click *Reports* and subsequently *Coupling* in the **View reports file** window.

For a complete overview of the graphical user interface of the Coupling module, see [sec-](#)

tion 5.2.

7.1.4 Preparing the water quality scenario

By clicking *Define input* in the **Water quality and ecology** selection window (Figure 4.3), the WAQ-GUI is started. The GUI guides you through the various input blocks required in the water quality modelling (Figure 5.16). After preparing all your water quality input, you can store your results in a scenario file (<*.scn>) by selecting *Save* or *Save As...* in the menu-item *File*. You can exit the WAQ-GUI by selecting *Exit* in the *File* menu-item.

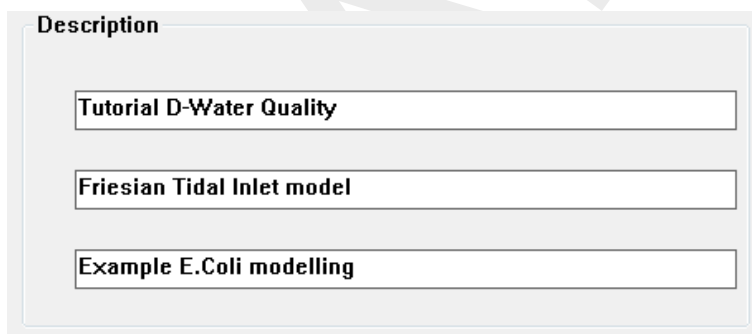
For every water quality calculation, you need to specify all data groups. For this tutorial case, this part of the tutorial guides you through these data groups.

7. PREPARING THE WATER QUALITY SCENARIO: START THE WATER QUALITY GUI

- ◇ In the **Water quality (WAQ)** selection window, click *Define input*.

7.1.4.1 Description

Three lines of 39 characters each can be used to specify some meta data. An example of this meta data is given in Figure 7.5.



The image shows a window titled 'Description' with three text input fields. The first field contains the text 'Tutorial D-Water Quality', the second field contains 'Friesian Tidal Inlet model', and the third field contains 'Example E.Coli modelling'.

Figure 7.5: Meta data displayed in the **Description** window

8. PREPARING THE WATER QUALITY SCENARIO: DESCRIPTION

- ◇ In the WAQ-GUI, click *Description*.
- ◇ Enter “Tutorial D-Water Quality” in the first line.
- ◇ Enter “Friesian Tidal Inlet model” in the second line.
- ◇ Enter “Example E.Coli modelling” in the third line.

An extensive description of the *Description* Data Group can be found in [section 5.3.1](#).

7.1.4.2 Hydrodynamics

In order to prepare a water quality simulation you must first select the coupled hydrodynamics. By clicking the *Select* button, you can browse to the <*.hyd> file, you just have coupled <tut_fti_waq.hyd>. By selecting this file and clicking *Open*, the details of the hydrodynamics are displayed: time information, horizontal and vertical aggregation. Note that you can only *inspect* the results of the hydrodynamic coupling here, no changes can be made. If you want

to, you should close this scenario and return to the coupling module again. Implement your changes there.

9. PREPARING THE WATER QUALITY SCENARIO: HYDRODYNAMICS

- ◇ In the WAQ-GUI, click *Hydrodynamics*.
- ◇ Click *Select*, browse to the <tut_fti_waq.hyd> file.
- ◇ Click *Open* to confirm.
- ◇ Inspect the displayed details of the hydrodynamics, see [Figure 7.6](#).

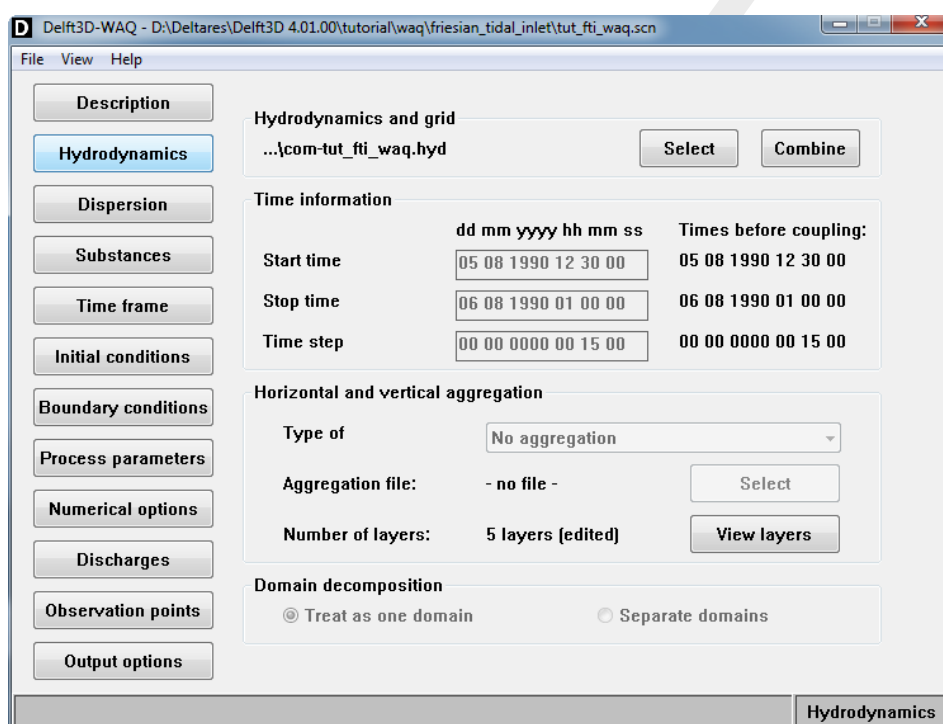


Figure 7.6: Data displayed in the *Hydrodynamics* window

An extensive description of the *Hydrodynamics* Data Group can be found in [section 5.3.2](#).

7.1.4.3 Dispersion

Dispersion coefficients are required to solve the advection-dispersion-reaction equation for water quality modelling. The default values for *Uniform dispersion* can be adapted. The *Additional vertical diffusion* coefficients can not be adapted. These coefficients are extracted from the hydrodynamic database by the coupling program. These diffusion (or dispersion) coefficients are called 'additional' since they are added to the uniform dispersion coefficients defined for the horizontal plane. *We advise you to set the uniform dispersion coefficient for the vertical direction to a low value (e.g. $1.0 \cdot 10^{-7}$) if for Additional vertical diffusion, Use results from hydrodynamics is selected.*

For the tutorial case, select the uniform dispersion by leaving the uniform default values untouched and specify *Use results from hydrodynamics* in the drop-down box in the *Additional vertical diffusion* frame.

10. PREPARING THE WATER QUALITY SCENARIO: DISPERSION

- ◇ In the WAQ-GUI, click *Dispersion*.
- ◇ Inspect and do not change the (default) uniform dispersion values.
- ◇ In the *Additional vertical diffusion* frame select *Use results from hydrodynamics*.
- ◇ See [Figure 7.7](#).

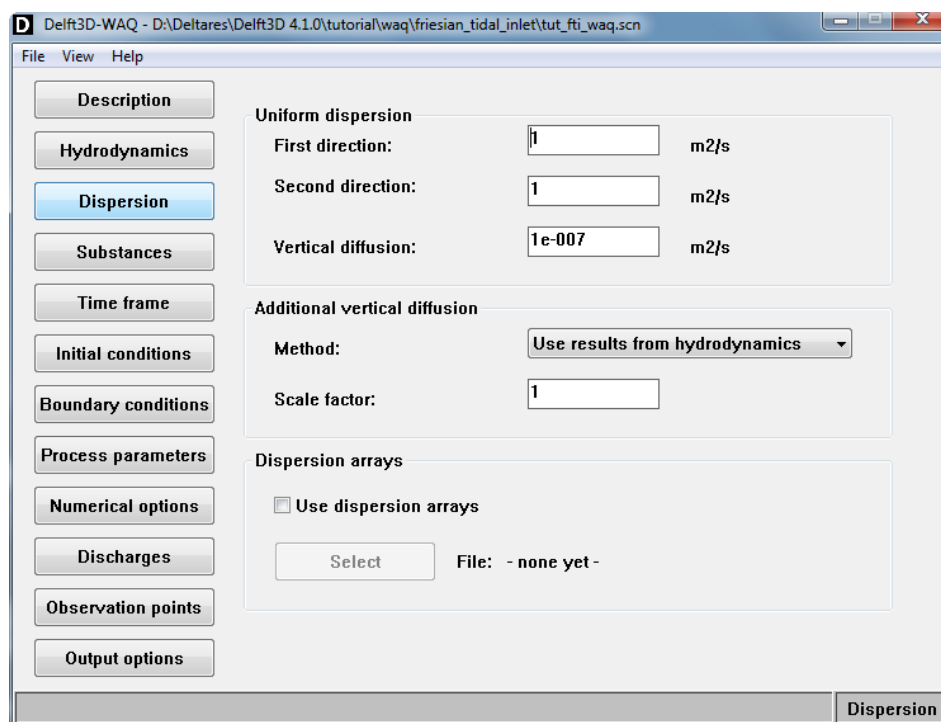


Figure 7.7: Datagroup *Dispersion* window

An extensive description of the *Dispersion* Data Group can be found in [section 5.3.3](#).

7.1.4.4 Substances

The substances and processes you want to model in your water quality calculation must be specified here. For the 'tut_fti_waq' tutorial case, a so-called *substance* file, describing E.Coli bacteria, is available. The corresponding filename is <coli_04.sub>. This file can be found in the <.../tutorial/waq/substances> directory. To import this file, click *Select* and browse to the mentioned directory, select the <coli_04.sub> file and click *Open*. The window as displayed in [Figure 7.8](#) will appear.

Of course, any other substance file created with the PLCT can be imported here. A separate part of this manual describes the PLCT in detail. More information about this tool can be found in [section 5.1](#). A descriptive document explaining mortality of E.Coli bacteria can be in [section B.3](#).

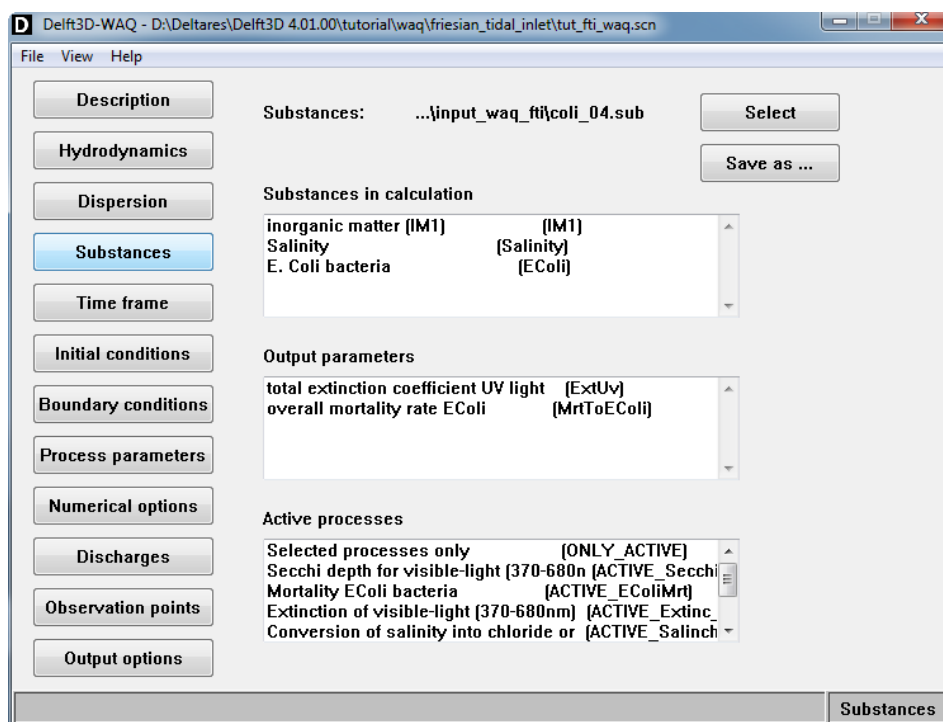


Figure 7.8: Data Group Substances showing <coli_04.sub>

11. PREPARING THE WATER QUALITY SCENARIO: SUBSTANCES

- ◇ In the WAQ-GUI, click *Substances*.
- ◇ Click *Select* and browse to the <.../tutorial/waq/substances> directory to select the <coli_04.sub> file.
- ◇ Click *Open* to confirm.
- ◇ Inspect the details which are loaded into the GUI, see [Figure 7.8](#)

An extensive description of the *Substances* Data Group can be found in [section 5.3.4](#).

7.1.4.5 Time frame

In this data group, you should specify the start time, stop time and time step of the water quality calculation. By default the values of the hydrodynamics are displayed. For the tutorial case, the start time is the same as for the hydrodynamics (05 08 1990 12 30 00) but the stop time should be changed to “15 08 1990 12 30 00”, so our calculation lasts for 10 days (the hydrodynamics will automatically be ‘repeated’ every 12.5 hours). The water quality time step remains 15 minutes. See [Figure 7.9](#).

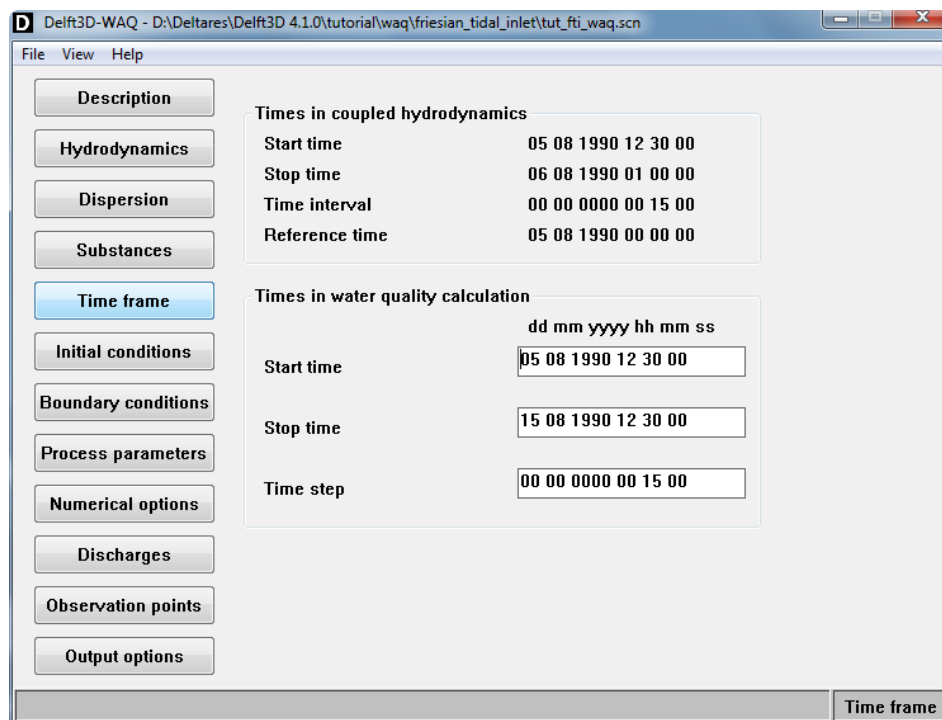


Figure 7.9: Time frame window

12. PREPARING THE WATER QUALITY SCENARIO: TIME FRAME

- ◇ In the WAQ-GUI, click *Time frame*.
- ◇ The content of the *Start time* entry box should be: "05 08 1990 12 30 00".
- ◇ The content of the *Stop time* entry box should be: "15 08 1990 12 30 00".
- ◇ The content of the *Timestep* entry box should be: "00 00 0000 00 15 00".
- ◇ See [Figure 7.9](#).

An extensive description of the *Time frame* Data Group can be found in [section 5.3.5](#).

7.1.4.6 Initial conditions

In this data group you specify starting (initial) conditions for all substances. Options are: a constant value (uniform value for the whole model area) or non-uniform values. The list of substances to be filled in, is automatically generated and originates from the selected `<*.sub>` file.

In our tutorial case, three initial conditions need to be specified: Salinity [g/kg], E.Coli bacteria [MPN/m³] and inorganic matter [gDM/m³]. We use uniform values for the substances. You can use the following values, see [Table 7.5](#).

Table 7.5: Initial Conditions

| Substance | Initial value [unit] | |
|------------------|----------------------|-----------------------|
| Salinity | 35 | [g/kg] |
| E.Coli bacteria | 0 | [MPN/m ³] |
| inorganic matter | 10 | [gDM/m ³] |

13. PREPARING THE WATER QUALITY SCENARIO: INITIAL CONDITIONS

- ◇ In the WAQ-GUI, click *Initial conditions*.
- ◇ Select the *inorganic matter* entry box and enter the value: “10”.
- ◇ Select the *Salinity* entry box and enter the value: “35”.
- ◇ Select the *E.Coli bacteria* entry box and enter the value: “0”.
- ◇ See [Figure 7.10](#).

| | |
|--|----|
| inorganic matter (IM1) (IM1; [gDM/m3]) | 10 |
| Salinity (Salinity; [g/kg]) | 35 |
| E. Coli bacteria (EColi; [MPN/m3]) | 0 |

Figure 7.10: Initial conditions window

An extensive description of the *Initial conditions* Data Group can be found in [section 5.3.6](#).

7.1.4.7 Boundary conditions

Boundary conditions are the concentrations of all active substances coming from the 'outside world' into the model area. These can vary in time, depth and location. Boundary conditions may have an important effect on the final model results. Therefore, the model grid schematisation should be large enough to prevent any unwanted concentration fluctuations resulting from these boundaries, or from irregularities in the hydrodynamic flows across these boundaries. In case the boundaries are far away from the area of interest of the modeller (a discharge location, an estuary, a harbour, a regional sea etc.) it usually suffices to take constant boundary conditions (obviously the constants should be chosen carefully). However, for studies over longer periods of time, time-dependent boundary conditions are often required.

For the tutorial case, in which we will focus on an E.Coli bacteria discharge, the boundary conditions are the same as the initial conditions, so the values in [Table 7.5](#) can be applied. Select *Boundary conditions* and select the *Left-right 1* boundary in the list. Click *Edit data* and fill in the values from [Table 7.5](#).

14. PREPARING THE WATER QUALITY SCENARIO: BOUNDARY CONDITIONS

- ◇ In the WAQ-GUI, click *Boundary conditions*.
- ◇ Select the *Left-right 1* from the list.

14. PREPARING THE WATER QUALITY SCENARIO: BOUNDARY CONDITIONS

To view the location of the open boundary

- ◇ Select menu-item *View* → *Visualise area* to open the **Visualisation Area** window.
- ◇ Select menu-item *Edit* and select *Open boundaries* (note that a round curved bold line will appear in blue or red).
- ◇ Close this window by selecting menu-item *File* → *Exit*.

To edit the Boundary conditions data

- ◇ Open or go back to the main *Boundary conditions* window.
- ◇ Select the *Left-right 1* from the list.
- ◇ Select *Edit data*.
- ◇ Select the *Salinity* entry box and enter the value: “35”.
- ◇ Select the *E.Coli bacteria* entry box and enter the value: “0”.
- ◇ Select the *IM1* entry box and enter the value: “10”.
- ◇ Select menu-option *Data* → *Save and exit* to save the data and return to the main window.
- ◇ See [Figure 7.11](#) for boundary conditions data.

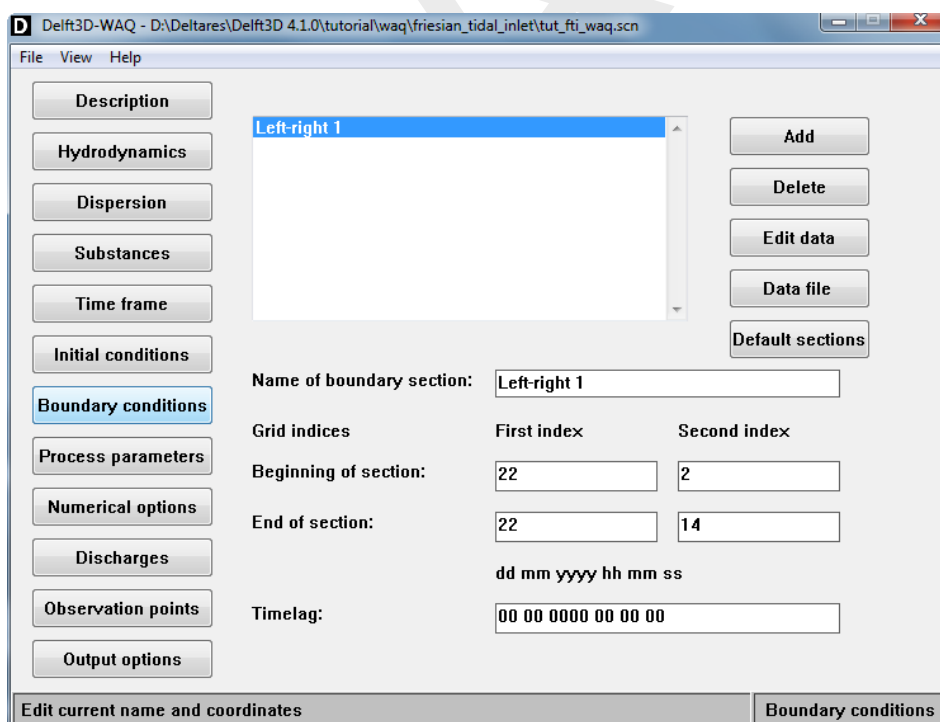


Figure 7.11: Boundary conditions window

An extensive description of the *Boundary conditions* Data Group can be found in [section 5.3.7](#).

7.1.4.8 Process parameters

In this data group the editable process parameters as selected within the Processes Library Configuration Tool will appear. For the tutorial case, you need the following values.

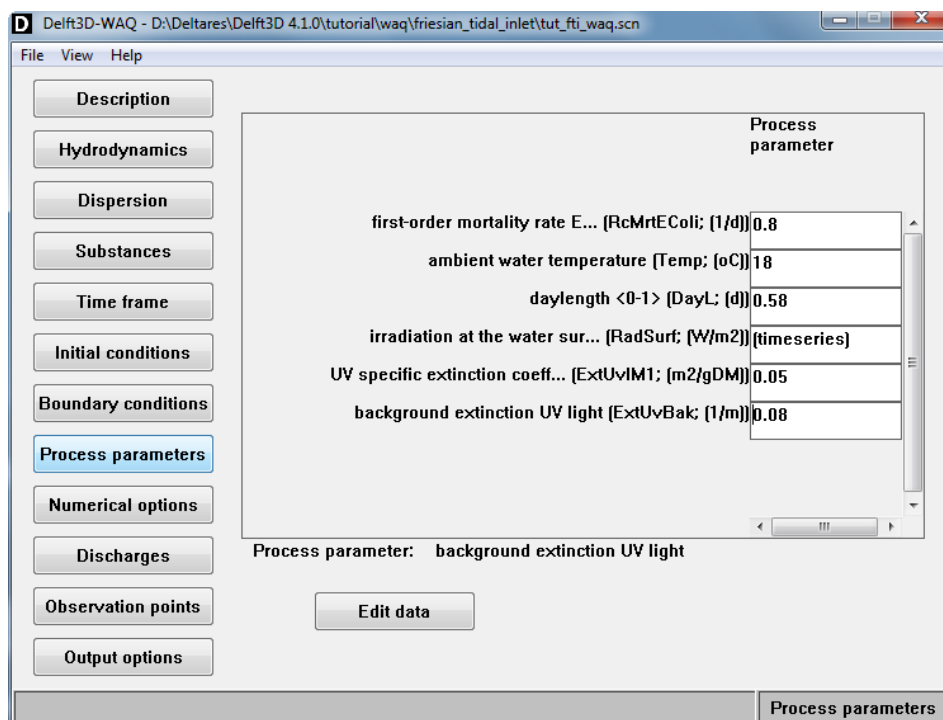


Figure 7.12: Data Group Process parameters

First the irradiation will be discussed (see row 4 in Figure 7.12) and then the other parameters.

Irradiation

Ultraviolet (UV) light increases the mortality of E.Coli bacteria. In summer, more UV light reaches the water surface so mortality will be higher. A more realistic approach for this parameter is a time-series. Summer values (during sunny circumstances) can reach up to 250 W/m² (total radiation). For the tutorial case, during a period of 10 days in August, the UV radiation varies between 190 (lower bound) and 250 W/m² (upper bound). You can create the time-series as follows:

In the *Process parameters* Data Group, select the parameter “irradiation at the water surface” by clicking the entry box behind the parameter. *Edit data* will be enabled. Clicking this button will bring up another window where you specify the data. Select menu-option *Properties* → *Data Properties* and check the radio button *Timeseries (block function)* in the *Time frame* (Figure 7.13).

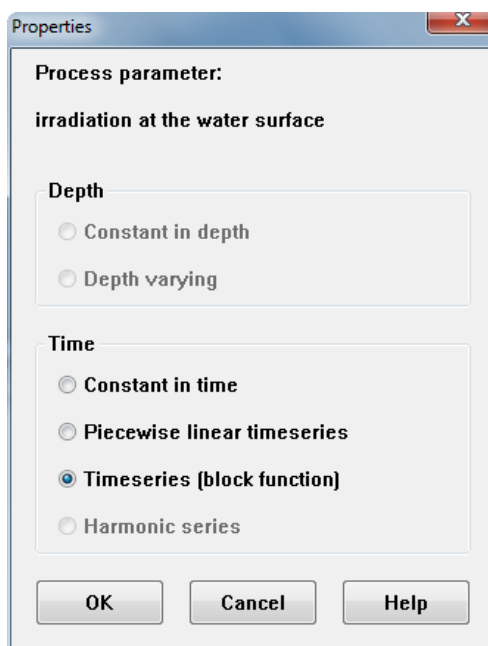


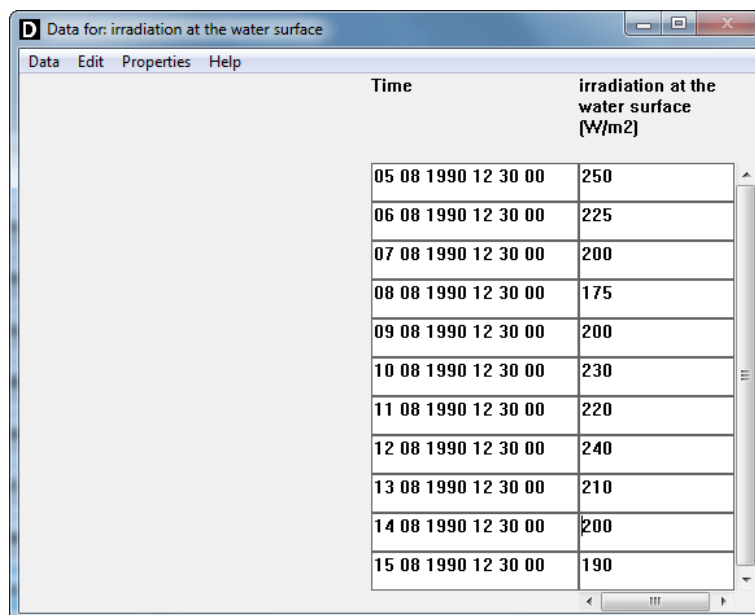
Figure 7.13: Specifying Timeseries in the **Properties** window

After confirming by pressing *OK*, the start time and stop time will appear in two different rows. Behind each time breakpoint you can specify a value for irradiation. By default these values are “-999” (*missing values*). See [Figure 7.14](#).

| Time | irradiation at the water surface [W/m2] |
|---------------------|---|
| 05 08 1990 12 30 00 | -999 |
| 15 08 1990 12 30 00 | -999 |

Figure 7.14: Time breakpoints in **Edit data** window after specifying Data Properties

To increase the number of breakpoints, select *Edit* → *Copy row*. The selected row will be copied. Use this option and change the content of the cells in such a way that it looks as in [Figure 7.15](#). Now every day in the calculation has its own irradiation value. After adding and editing rows, select menu-option *Data* → *Save and exit*. Now the window as in [Figure 7.12](#) will appear again. The entry box behind *irradiation at the water surface* will indicate “[timeseries]”.



The screenshot shows a window titled "D Data for: irradiation at the water surface" with a menu bar (Data, Edit, Properties, Help). It contains a table with two columns: "Time" and "irradiation at the water surface [W/m2]". The table lists 11 rows of data for the dates 05 to 15 of August 1990 at 12:30:00.

| Time | irradiation at the water surface [W/m2] |
|---------------------|---|
| 05 08 1990 12 30 00 | 250 |
| 06 08 1990 12 30 00 | 225 |
| 07 08 1990 12 30 00 | 200 |
| 08 08 1990 12 30 00 | 175 |
| 09 08 1990 12 30 00 | 200 |
| 10 08 1990 12 30 00 | 230 |
| 11 08 1990 12 30 00 | 220 |
| 12 08 1990 12 30 00 | 240 |
| 13 08 1990 12 30 00 | 210 |
| 14 08 1990 12 30 00 | 200 |
| 15 08 1990 12 30 00 | 190 |

Figure 7.15: Irradiation values for the 10-day calculation

Other parameters

Specify the other parameters like in [Figure 7.12](#):

- ◇ first-order mortality rate E.Coli: "0.8"
- ◇ ambient water temperature: "18"
- ◇ daylength [0,1]: "0.58"
- ◇ UV specific extinction coefficient IM1: "0.05"
- ◇ background extinction UV light: "0.08"

15. PREPARING THE WATER QUALITY SCENARIO: PROCESS PARAMETERS

- ◇ In the WAQ-GUI, click *Process parameters*.

Time-series for Irradiation at the water surface

- ◇ Select the "irradiation at the water surface" entry box.
- ◇ Click *Edit data*.
- ◇ Select menu-option *Properties* → *Data Properties* and specify the radio button *Time-series (block function)* in the *Time* frame.
- ◇ Increase the number of breakpoints to 11 by using menu-option *Edit* → *Copy row* or *Ctrl+K* several times.
- ◇ Update the content of the 11-row table according to [Figure 7.15](#).
- ◇ Select menu-option *Data* → *Save and exit* to confirm your time-series.

Other process parameters

- ◇ Select the other five entry boxes individually and enter the corresponding values displayed in [Figure 7.12](#).

An extensive description of the *Process parameters* Data Group can be found in [section 5.3.8](#).

7.1.4.9 Numerical options

In this data group you must specify the integration method (numerical scheme) with which you want to carry out your water quality calculation. In the tutorial case, please select integration method 16 from the drop-down box. Check the two checkboxes in the *Dispersion* frame and the one in the *Transport over boundaries* frame. Your window should look like as in [Figure 7.16](#).

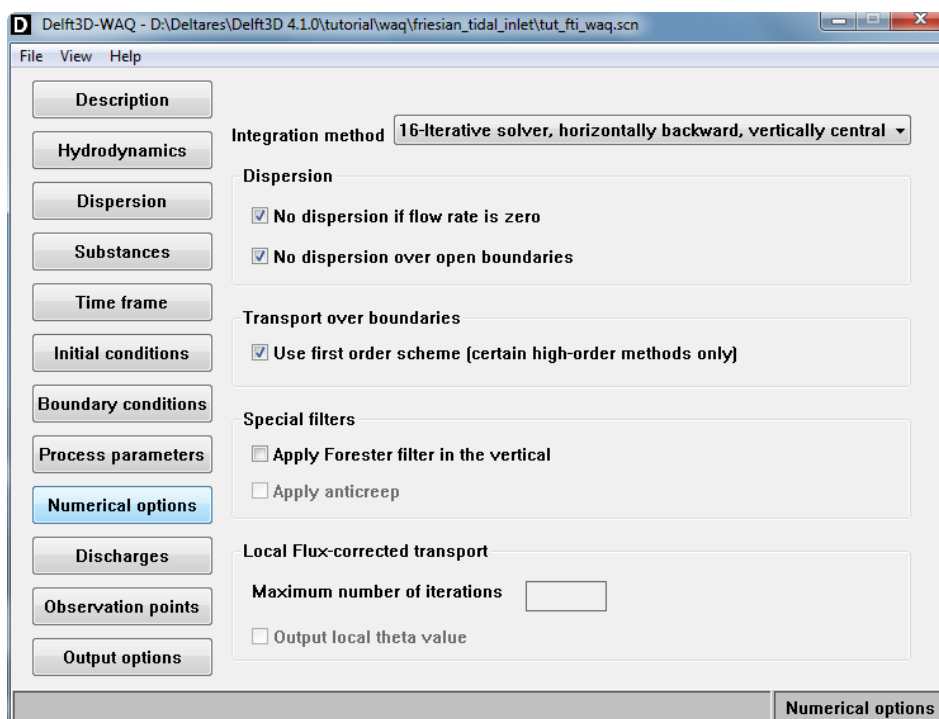


Figure 7.16: Numerical options for tutorial case

16. PREPARING THE WATER QUALITY SCENARIO: NUMERICAL OPTIONS

- ◇ In the WAQ-GUI, click *Numerical options*.
- ◇ Select the “16-iterative solver, horizontally backward, vertically central” from the *Integration method* drop-down box.
- ◇ In the *Dispersion* frame, check the “No dispersion if flow rate is zero” check box.
- ◇ In the *Dispersion* frame, check the “No dispersion over open boundaries” check box.
- ◇ In the *Transport over boundaries* frame, check the “Use first order scheme (certain high-order methods only)” check box.
- ◇ See [Figure 7.16](#).

An extensive description of the *Numerical options* Data Group can be found in [section 5.3.9](#).

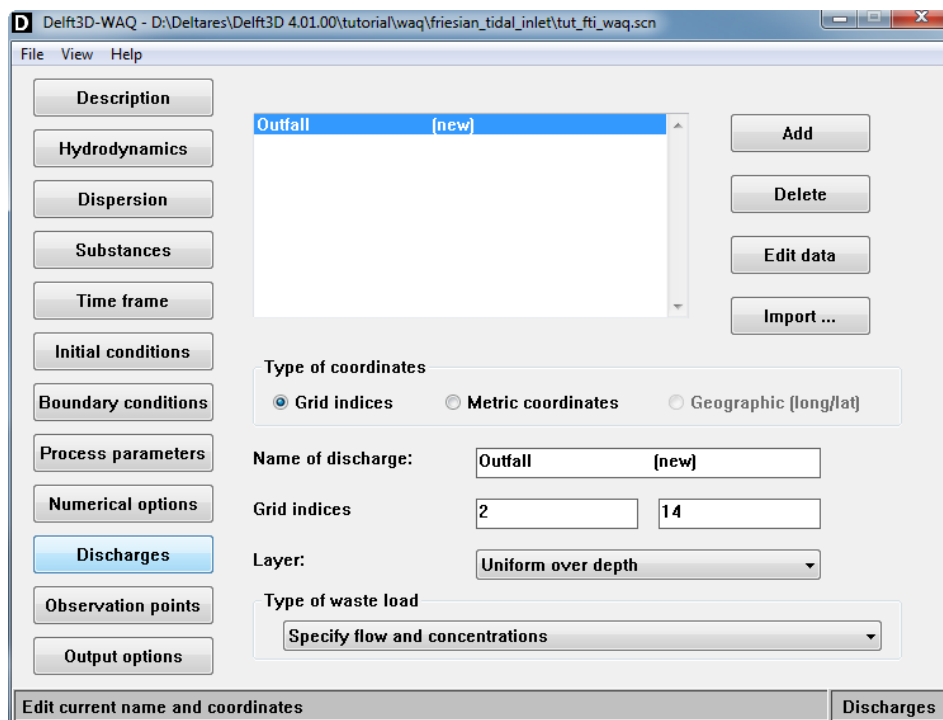


Figure 7.17: Discharges converted by the Coupling module

7.1.4.10 Discharges

In this data group you will specify the E.Coli discharge in the tutorial case. The location of a discharge can be pointed by using the **Visualisation Area** or specifying grid indices. Both options are explained. Another possibility is that discharges already defined in the hydrodynamics are imported through the WAQ-GUI. They will be visible in the discharges list when you select the hydrodynamic results.

Discharges from hydrodynamics

If the hydrodynamic database already contains one or more discharges, these will be converted by the coupling module. If you load these results into the water quality scenario (Data Group *Hydrodynamics*) these (pre)defined discharges will be available in the GUI (see Figure 7.17). The discharge is called “Outfall (new)”.

If you select this name in the list, additional details appear in the lower part of the window. Select the entry box behind *Name of discharge* and change it into “E.Coli discharge”.

- ◇ *Create a new discharge by location specification using the Visualisation Area*
Use menu-option **View** → **Visualise area** to open the **Visualisation Area** window. In this window, use the menu-option **Edit** to check the **Discharges** menu-item. Use the **Edit Mode** menu-option to check **Add**. In this mode you can select a location in the grid to pinpoint a discharge location. A red diamond will appear in the selected grid cell. The **Discharges** Data Group window will be updated with this discharge. Details can be specified in this window.
Move your mouse to the opening between the two islands (first and second indices change at the right-top side of the screen) towards location *first index* = 8 and *second index* = 14, click here and a red diamond appears. Go back to the data group window and change the *Name of discharge* to “IM1 discharge”.
- ◇ *Create a new discharge by location specification using the Add button and grid indices*

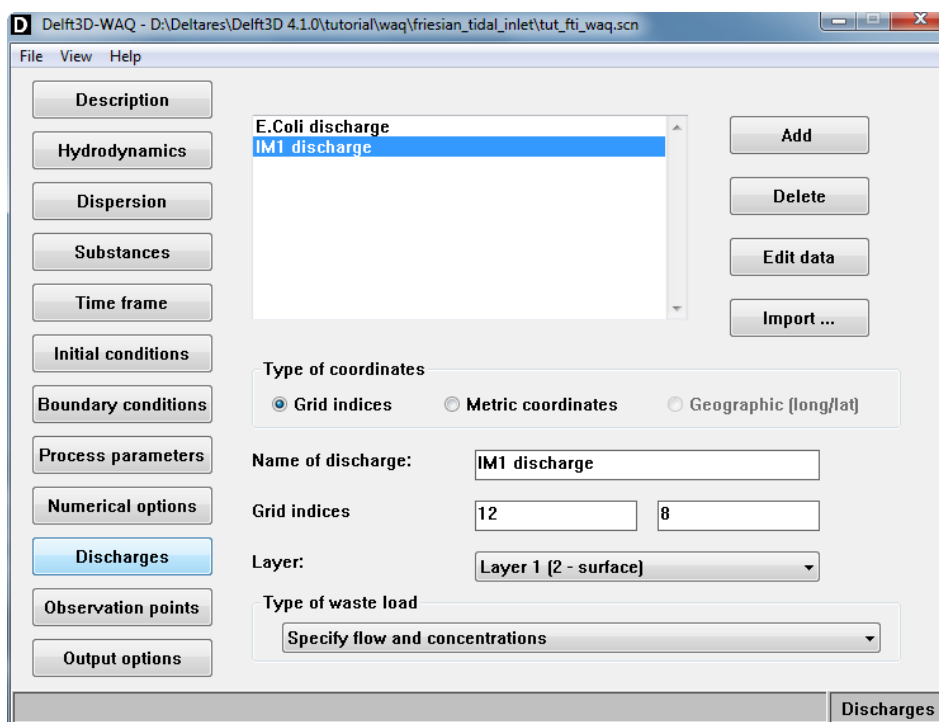


Figure 7.18: Discharges Data Group including the E.Coli discharge and the IM1 discharge

In the Data Group *Discharges* window you can press *Add*. A new discharge appears in the list. Details of this discharge can be specified in the lower half of the window. The *Grid indices* needs to be button. Enter “12” in the left box and “8” in the right box. Change the *Name of discharge* to “IM1 discharge”.

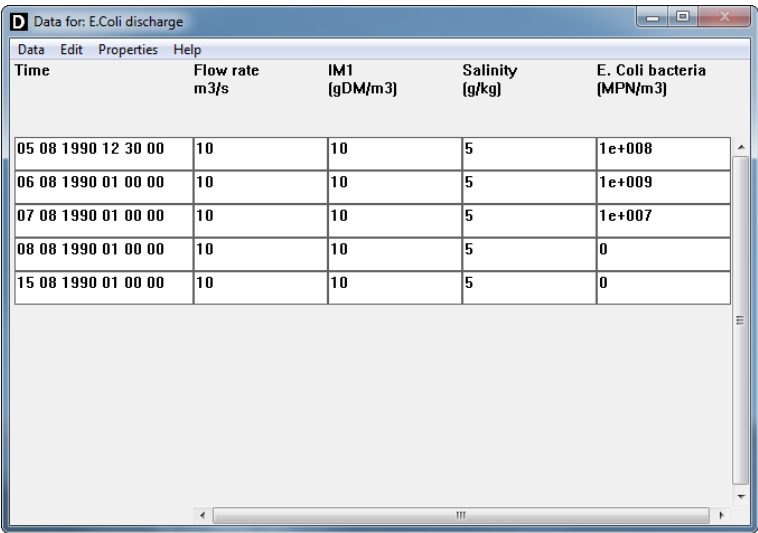
The results should look like [Figure 7.18](#).

- | | |
|------------------|--|
| Discharge height | The E.Coli discharge is in the surface layer, so the <i>Layer</i> drop-down box should indicate “Uniform over depth”. For the IM1 discharge choose “Layer 1 (2-surface)”. |
| Discharge data | Select the <i>E.Coli discharge</i> in the list and click <i>Edit data</i> . Select menu-option <i>Properties</i> → <i>Data Properties</i> and check the radio button <i>Timeseries (block function)</i> in the <i>Time frame</i> . Just like in <i>Process parameters</i> (Irradiation) you can specify a time-series for the load of this E.Coli bacteria discharge. For each time breakpoint you should specify discharge data for each substance (in our case: Salinity, E.Coli and IM1). Flow rates are coming from the hydrodynamic database and are set constant to $3 \text{ m}^3 \text{ s}^{-1}$. |

Click in one of the entry boxes of time breakpoint table and use menu-option *Edit* → *Copy row* to increase the number of rows. Repeat this action and change the content until it looks like [Figure 7.19](#).

Select *Data* → *Save and exit* to store your entered discharge rates for the E.Coli discharge.

Select the *IM1 discharge* in the list and click *Edit data*. Select menu-option *Properties* → *Data Properties* and check the radio button *Constant in time* in the lower frame (*Time*). For each substance (in our case: Salinity, E.Coli and IM1) you can specify a (constant) value. If



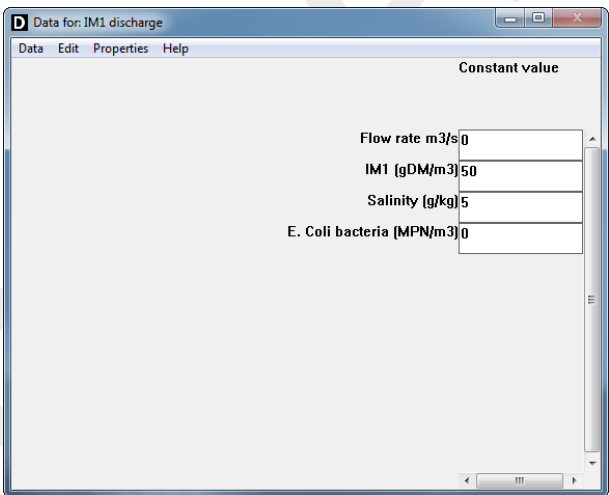
| Time | Flow rate m3/s | IM1 (gDM/m3) | Salinity (g/kg) | E. Coli bacteria (MPN/m3) |
|---------------------|-------------------|-----------------|--------------------|------------------------------|
| 05 08 1990 12 30 00 | 10 | 10 | 5 | 1e+008 |
| 06 08 1990 01 00 00 | 10 | 10 | 5 | 1e+009 |
| 07 08 1990 01 00 00 | 10 | 10 | 5 | 1e+007 |
| 08 08 1990 01 00 00 | 10 | 10 | 5 | 0 |
| 15 08 1990 01 00 00 | 10 | 10 | 5 | 0 |

Figure 7.19: Discharge data of the E.Coli discharge

you leave *Flow rate* [m³/s] zero, the values will be interpreted as ‘loads’ (mass/time). Use the values as displayed in [Figure 7.20](#).

Select *Data* → *Save and exit* to store your entered discharge rates for the IM1 discharge.

Leave the *Type of waste load* on the default selection *Specify flow and concentrations*



Constant value

Flow rate m3/s 0

IM1 (gDM/m3) 50

Salinity (g/kg) 5

E. Coli bacteria (MPN/m3) 0

Figure 7.20: Discharge data of the IM1 discharge

17. PREPARING THE WATER QUALITY SCENARIO: DISCHARGES

- ◇ In the WAQ-GUI, click *Discharges*

Editing details of imported discharges (from Coupling module)

- ◇ The (only) discharge coming from the Coupling module is called: “outfall (new)”.
- ◇ Click the name in the list;
- ◇ Select the *Name of discharge* entry box and change the name into “E.Coli discharge”.
- ◇ Click *Edit data*.
- ◇ Select menu-option *Properties* → *Data Properties* and check the radio button *Time-series (block function)* in the *Time* frame.
- ◇ Increase the number of breakpoints to 5 by using menu-option *Edit* → *Copy row* several times.
- ◇ Update the content of the 5-row table according to [Figure 7.19](#).
- ◇ Select menu-option *Data* → *Save and exit* to confirm your discharge data.

Adding the discharge by using the Visualisation Area window

- ◇ Use menu-option *View* → *Visualise area* to open the **Visualisation Area** window.
- ◇ In the **Visualisation Area** window, select *Discharges* from the *Edit* menu and *Add* from the *Edit Mode* menu.
- ◇ Move your mouse to the cell with indices *first index* = 12 and *second index* = 8 (somewhere in between the two islands) and click your left mouse.
- ◇ Return to the main Discharges window (and close the **Visualisation Area** by using menu-option *File* → *Exit*).

or

Adding the discharge by using the Add button/Grid indices

- ◇ Click *Add* and enter “12” in the *left Grid indices* entry box and “8” in the *right Grid indices* entry box.

and

Specifying other details

- ◇ Select the just added discharge from the list.
- ◇ Enter “IM1 discharge” in the *Name of discharge* entry box.
- ◇ Specify *Layer 1 (2 - surface)* from the *Layer* drop-down box.
- ◇ Click *Edit data*.
- ◇ Select menu-option *Properties* → *Data Properties* and check the radio button *Constant in time* in the *Time* frame.
- ◇ Update the content of the table according to [Figure 7.20](#).
- ◇ Select menu-option *Data* → *Save and exit* to confirm your discharge data.
- ◇ Specify *Specify flow and concentrations* from the *Type of waste load* drop-down box.

An extensive description of the *Discharges* Data Group can be found in [section 5.3.10](#).

7.1.4.11 Observation points

To assess the water quality calculation, you need to specify observation points for which output will be stored. First you have to pinpoint the location of these observation points in the grid.

Table 7.9: Settings for the 4 observation points.

| Name | Layer | first index | second index |
|-------------|--------------------|-------------|--------------|
| left upper | Separate per layer | 16 | 6 |
| right upper | Separate per layer | 16 | 11 |
| left lower | Separate per layer | 8 | 6 |
| right lower | Separate per layer | 8 | 11 |

Like the discharges you can specify the location by either using the **Visualisation Area** or using *Add* and the *Grid indices* boxes.

◇ *Defining observation points using the Visualisation Area*

Open the **Visualisation Area** from the menu-option *View* → *Visualise area*. In this window, use the menu-option *Edit* → *Observation points*. Use the *Edit Mode* menu-option to check *Add*. In this mode you can select a location in the grid to pinpoint an observation point. A red cross will appear in the selected grid cell. The main data group window will be updated with this new observation point. Details, like name and layer can be specified here.

◇ *Location specification using the Add button and grid indices*

In the main data group window you can press *Add*. A new observation point appears in the list. Details of this discharge can be specified in the lower half of the window. The *Grid indices* need to be specified. Enter “16” in the left box and “6” in the right box. Change *Observation point* to “left upper”.

Observation point height

Like discharges, you can specify a layer for an observation point. Use the drop-down box to select a layer. If you want to have observation points in every layer, please select *Separate per layer*. The result is that you will get as many observation points as there are layers. The tutorial case has 5 water quality layers, so 5 observation points will be created in the selected grid cell.

Repeat this procedure until you have 4 observation points which comply with the settings in [Table 7.9](#).

The data group window, including the **Visualisation Area** looks like displayed in [Figure 7.21](#).

18. PREPARING THE WATER QUALITY SCENARIO: OBSERVATION POINTS

- ◇ In the WAQ-GUI, click *Observation points*.

18. PREPARING THE WATER QUALITY SCENARIO: OBSERVATION POINTS

Adding 4 observation points by using the Visualisation Area window

- ◇ Use menu-option *View* → *Visualise area* to open the **Visualisation Area** window.
- ◇ In the **Visualisation Area** window, select *Observation points* from the *Edit* menu and *Add* from the *Edit Mode* menu.
- ◇ Move your mouse to the cell with co-ordinates *first* = 16 and *second* = 6 and click your left mouse.
- ◇ Move your mouse to the cell with co-ordinates *first* = 16 and *second* = 11 and click your left mouse.
- ◇ Move your mouse to the cell with co-ordinates *first* = 8 and *second* = 6 and click your left mouse.
- ◇ Move your mouse to the cell with co-ordinates *first* = 8 and *second* = 11 and click your left mouse.
- ◇ Return to the main *Observation points* window.

or

Adding 4 observation points by using the Add button/Grid indices

- ◇ Click *Add* and enter “16” in the left *Grid indices* entry box and “6” in the right *Grid indices* entry box.
- ◇ Click *Add* and enter “16” in the left *Grid indices* entry box and “11” in the right *Grid indices* entry box.
- ◇ Click *Add* and enter “8” in the left *Grid indices* entry box and “6” in the right *Grid indices* entry box.
- ◇ Click *Add* and enter “8” in the left *Grid indices* entry box and “11” in the right *Grid indices* entry box.

and

Specifying other details

- ◇ Select the (just added) first observation point from the list.
- ◇ Enter “left upper” in the *Observation point* entry box.
- ◇ Select *Separate per layer* from the *Layer* drop-down box.
- ◇ Select the second observation point from the list.
- ◇ Enter “right upper” in the *Observation point* entry box.
- ◇ Select *Separate per layer* from the *Layer* drop-down box.
- ◇ Select the third observation point from the list.
- ◇ Enter “left lower” in the *Observation point* entry box.
- ◇ Select *Separate per layer* from the *Layer* drop-down box.
- ◇ Select the (just added) first observation point from the list.
- ◇ Enter “right lower” in the *Observation point* entry box.
- ◇ Select *Separate per layer* from the *Layer* drop-down box.
- ◇ Close the **Visualisation Area** by selecting menu-option *File* → *Exit*.

An extensive description of the *Observation points* Data Group can be found in [section 5.3.11](#).

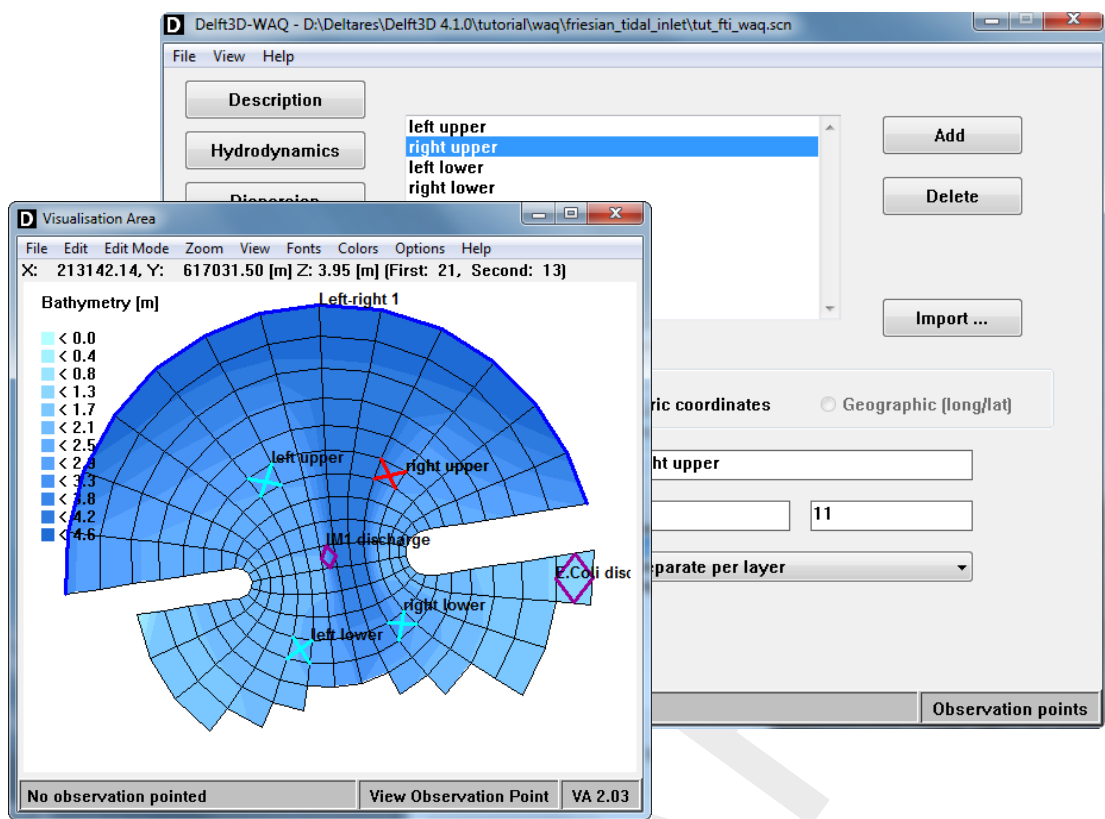


Figure 7.21: Observation points (crosses), discharge location (diamond) and open boundary (bold line)

| Type | Start time dd mm yyyy hh mm ss | Stop time dd mm yyyy hh mm ss | Time interval dd mm yyyy hh mm ss |
|---------|-----------------------------------|----------------------------------|--------------------------------------|
| Monitor | 05 08 1990 12 30 00 | 15 08 1990 12 30 00 | 00 00 0000 06 00 00 |
| History | 05 08 1990 12 30 00 | 15 08 1990 12 30 00 | 00 00 0000 01 00 00 |
| Map | 05 08 1990 12 30 00 | 15 08 1990 12 30 00 | 00 00 0000 02 00 00 |

Figure 7.22: Output Options - Timers

7.1.4.12 Output options

In this last data group you can specify the output. You can specify a selection of: output timers, output parameters, statistics, file types and formats.

Timers

You can specify the start and stop time of the output by changing the corresponding entry boxes. The time interval can be adjusted as well. You can specify different settings for the different file types. Change the text boxes according to [Figure 7.22](#).

Select output file types and formats

The following file types are available:

- ◇ Monitor file: ASCII output for the observation points;
- ◇ History file: time-series output of the observation points;
- ◇ Map file: geographical plots of concentration contours;
- ◇ Mass balance file: write a mass balance file.

The available formats are binary (unformatted) and NEFIS, for both windows and LINUX operating systems. Click *Files* to check the output files and types according to Figure 7.23.

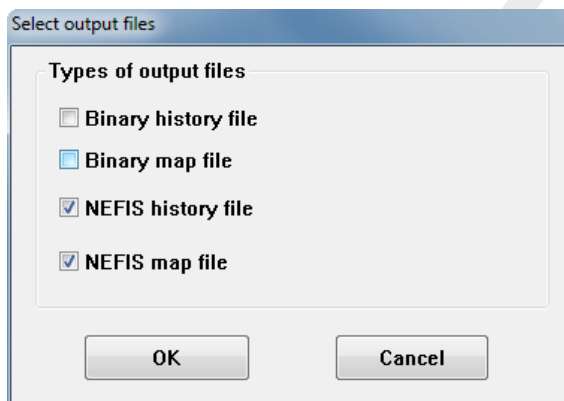


Figure 7.23: Select Output options → Files, showing window **Select output files**

Select parameters

The output parameters (defined in the PLCT) can be switched *on* (written to output files) or *off* (not written to output files). Click *Select* to specify this for every substance and file. See Figure 7.24.

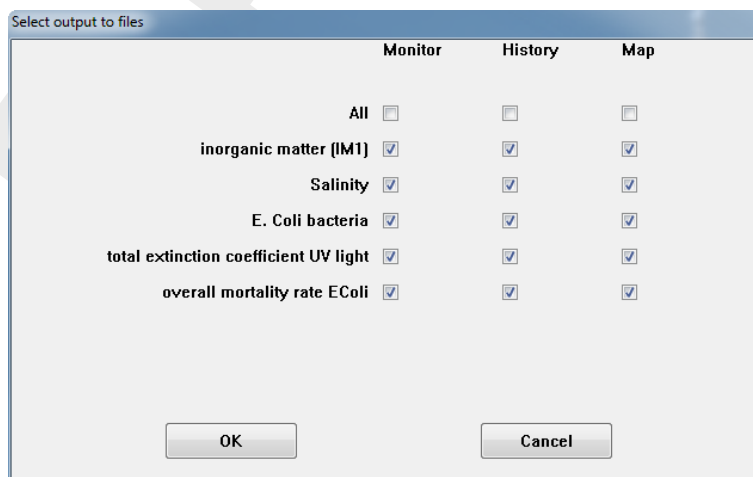


Figure 7.24: Select Output options → Select, showing window **Select output to files**

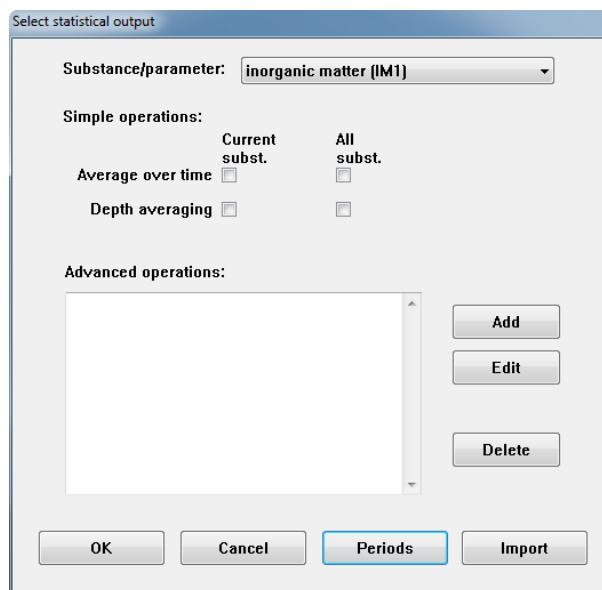


Figure 7.25: Window *Select statistical output*

Select statistics

Open the statistics window see [Figure 7.25](#).

- ◇ Click *Statistics*.
- ◇ Select the *All* checkbox in the *Average over time* column and
- ◇ Select the *All* checkbox in the *Depth averaging* column.
- ◇ Select the E.Coli bacteria substance; next click the *Periods* button.
- ◇ Click *Add*.
- ◇ Enter "whole period" in the *Name of period* entry box.
- ◇ Enter "whole" in the *Abbreviation* entry box.
- ◇ Enter "05 08 1990 12 30 00" in the *Start time* entry box.
- ◇ Enter "15 08 1990 12 30 00" in the *Stop time* entry box.
- ◇ Click *OK* to confirm.

First you need to define the period for which you like to have the statistics. Click the *Periods* button and press *Add*. Specify the "Whole period" as a period and "Whole" as abbreviation according to the settings in [Figure 7.26](#). Close this window by clicking *OK*.

Figure 7.26: Statistics - period definition

Check the *All* checkbox in the columns for *Average over time* and *Depth averaging* to select all available statistics for the output parameters.

Select *Substance/parameter* E.Coli bacteria. Click *Add* in the *Advanced operations* list box. Select *Periodic averages* from the *Statistical operation* drop-down box. Enter the *Suffix* “daily”. Specify the *Start time* as “05 08 1990 12 30 00” and set *Period* to 1 day (you will get daily averages now) by specifying “01 00 0000 00 00 00”. See [Figure 7.27](#) and then press *OK*.

Figure 7.27: Advanced statistics - Periodic averages

Click *Add* again. Select *Geometric mean* from the *Statistical operation* drop-down box. Enter the *Suffix* “geomean”. Specify *Threshold* as “1” (to prevent zero and negative values to be

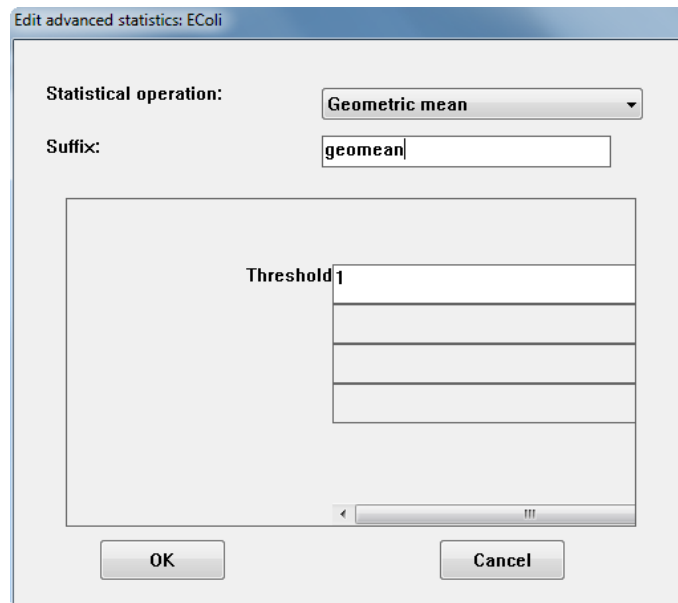


Figure 7.28: Advanced statistics - Geometric mean

included in the logarithmical calculations). See [Figure 7.28](#).

Close this window ([Figure 7.28](#)) by clicking *OK* and close the window **Select statistical output** ([Figure 7.25](#)) as well by clicking *OK*.

Balances

- Click the *Balances* button.
- Switch *on* the *Mass balances* radio buttons.
- Click *OK* to confirm and close the **Balances** window.

19. PREPARING THE WATER QUALITY SCENARIO: OUTPUT OPTIONS

- ◇ In the WAQ-GUI, click *Output options*.

Timers

- ◇ The content of the 3 *Start time* entry boxes should be: "05 08 1990 12 30 00".
- ◇ The content of the 3 *Stop time* entry boxes should be: "15 08 1990 12 30 00".
- ◇ The content of the 3 *Time interval* entry boxes should be:
 - Monitor file: "00 00 0000 06 00 00"
 - History file: "00 00 0000 01 00 00"
 - Map file: "00 00 0000 02 00 00"

Files

- ◇ Click *Files*.
- ◇ Switch off both *binary files* checkboxes.
- ◇ Switch on both *NEFIS files* checkboxes.
- ◇ Click *OK* to confirm.

Parameters

- ◇ Click *Select*.
- ◇ Select all output parameters for all 3 file types (3 times the *all* checkbox will ease this operation).
- ◇ Click *OK*

Statistics

- ◇ Click *Statistics*
- ◇ Check the *All* checkboxes and Substance parameter E.Coli
- ◇ Click *OK*
- ◇ Click *Add* in the *Advanced operations* frame.
- ◇ Select *Periodic averages* from the *Statistical operation* drop-down box.
- ◇ Enter "daily" in the *Suffix* entry box.
- ◇ Enter "05 08 1990 12 30 00" in the *Start time* entry box.
- ◇ Enter "01 00 0000 00 00 00" in the *Period* entry box.
- ◇ Click *OK* to confirm.
- ◇ Click *Add* in the *Advanced operations* frame.
- ◇ Select *Geometric mean* from the *Statistical operation* drop-down box.
- ◇ Enter "geomean" in the *Suffix* entry box.
- ◇ Click *OK* to confirm.
- ◇ Click *OK* to confirm and close the **Statistics** window.

Balances

- ◇ Click the *Balances* button.
- ◇ Switch *on* the *Mass balances* radio buttons.
- ◇ Click *OK* to confirm and close the **Balances** window.

An extensive description of the *Output options* Data Group can be found in [section 5.3.12](#).

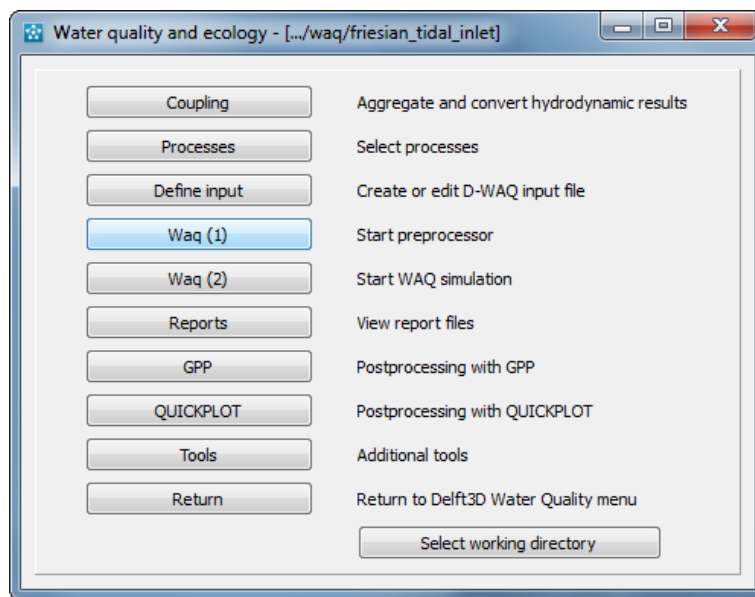


Figure 7.29: Water quality and ecology selection window

Saving the scenario file

From the WAQ-GUI, select menu-option File → Save or Save As to save your scenario file. Automatically the extension `<*.scn>` will be given. Save your file into the current working directory. All your results will be stored here as well.

The definition of the 'tut_fti_waq' tutorial case is ready now. Select menu-option File → Exit to exit the main window.

20. PREPARING THE WATER QUALITY SCENARIO: SAVING AND EXITING

Saving the scenario file

- ◇ In the WAQ-GUI, select menu-option File → Save or Save As to save your settings to a file. Name it `<tut_fti_waq.scn>` and store it in your *current working directory* (default location).

Exiting the WAQ-GUI

- ◇ In the WAQ-GUI, select menu-option File → Exit to quit.

7.1.5 Running the 'tut_fti_waq' scenario

The model has been set-up. It is ready to run now. The calculations consists of two parts: pre-processing and calculation (see Sections 6.1.1 and 6.1.4).

After exiting the WAQ-GUI (previous step) the window from Figure 7.29 appears. Click *Waq (1)*.

Press *Select file* and browse to the `<tut_fti_waq.inp>` file. This is the *input* file generated from your just saved `<tut_fti_waq.scn>` file. You can find them in your *current working directory*. Click *Open* to confirm. The window should look as in Figure 7.30.

After selecting *OK* the pre-processing program (delwaq1) will run to verify and process the input in a new window, see Figure 7.31. The program will end with a 'Normal end'.

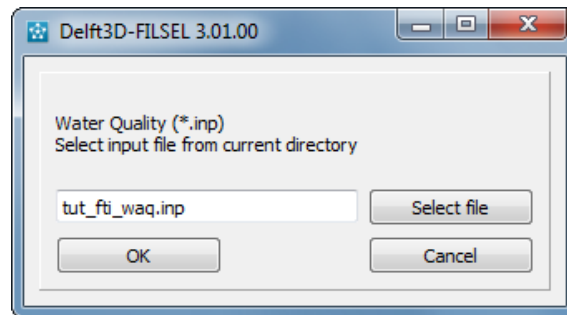


Figure 7.30: *Waq (1) - Pre-processing file selection*

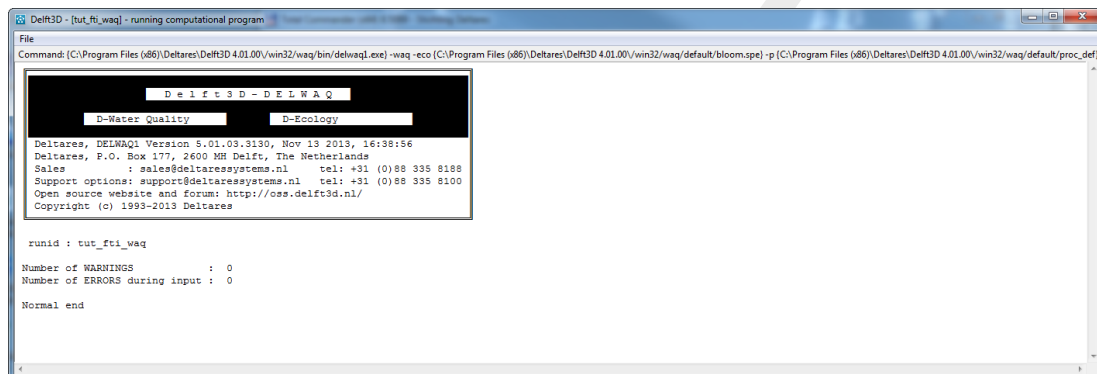


Figure 7.31: *Waq (1) window; pre-processing finished with 'Normal end'*

By pressing the *Waq (2)* button, the water quality calculation starts in a new window, see [Figure 7.32](#). The progress is monitored by displaying the percentage completed.

21. RUNNING THE WATER QUALITY SCENARIO

Running pre-processors

- ◇ In the **Water quality (WAQ)** window, click *Waq (1)*. Click *Select file* in the next window to select the <tut_fti_waq.inp> file.
- ◇ Click *OK* to confirm.
- ◇ The pre-processors will run in a new window.

Executing the water quality calculation

- ◇ Click *Waq (2)*. The calculation will start in a new window.

Close both windows by clicking *File* → *Exit* in each window.

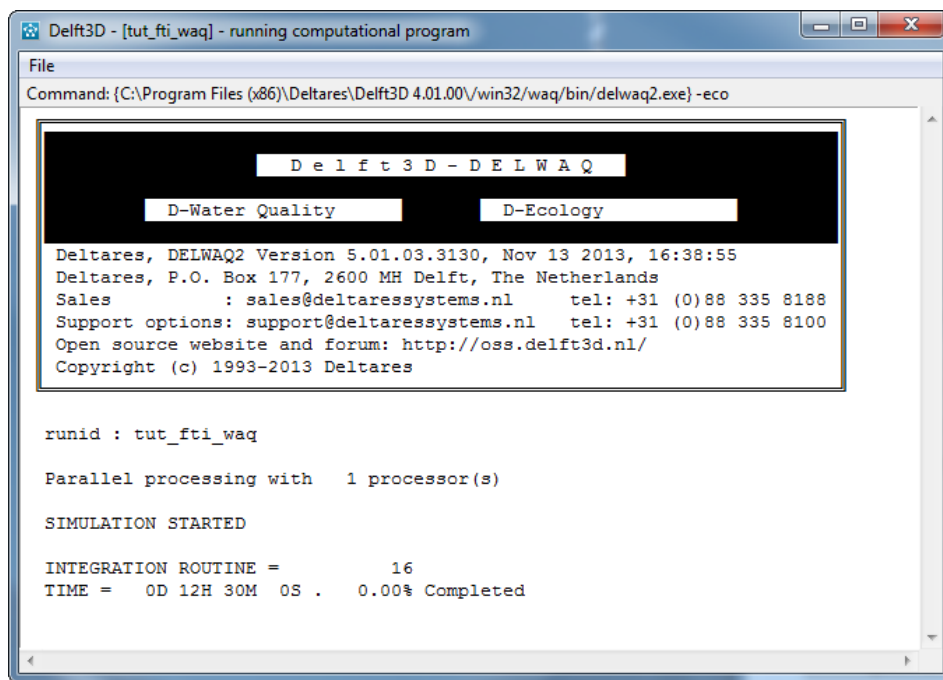


Figure 7.32: Waq (2) window showing the progress of the calculation.

7.1.6 Visualising results

To view output of a WAQ simulation, the GPP (General Post Processing) program can be used. By selecting **GPP** in the **Water quality (WAQ)** selection window (Figure 7.29), GPP starts. To open the so-called session file (<*.ssn>), the data sets and plots of the tutorial example will be opened. The session file to open is <tut_fti_waq.ssn> and can be found in the <\delft3d\tutorial\waq\friesian_tidal_inlet> directory. Use the menu-item *Session* → *Open...* (select *No* if you are asked to save changes) to browse to the <tut_fti_waq.ssn> file, click *Open* to confirm.

The plots can be found when you click *Plots*. Select a plot from the list and click the *View/Edit* to open it. Figure 7.33 till Figure 7.37 are examples of figures presenting water quality parameters from the tutorial case. See the GPP User Manual (GPP UM, 2013) for details on how to use GPP.

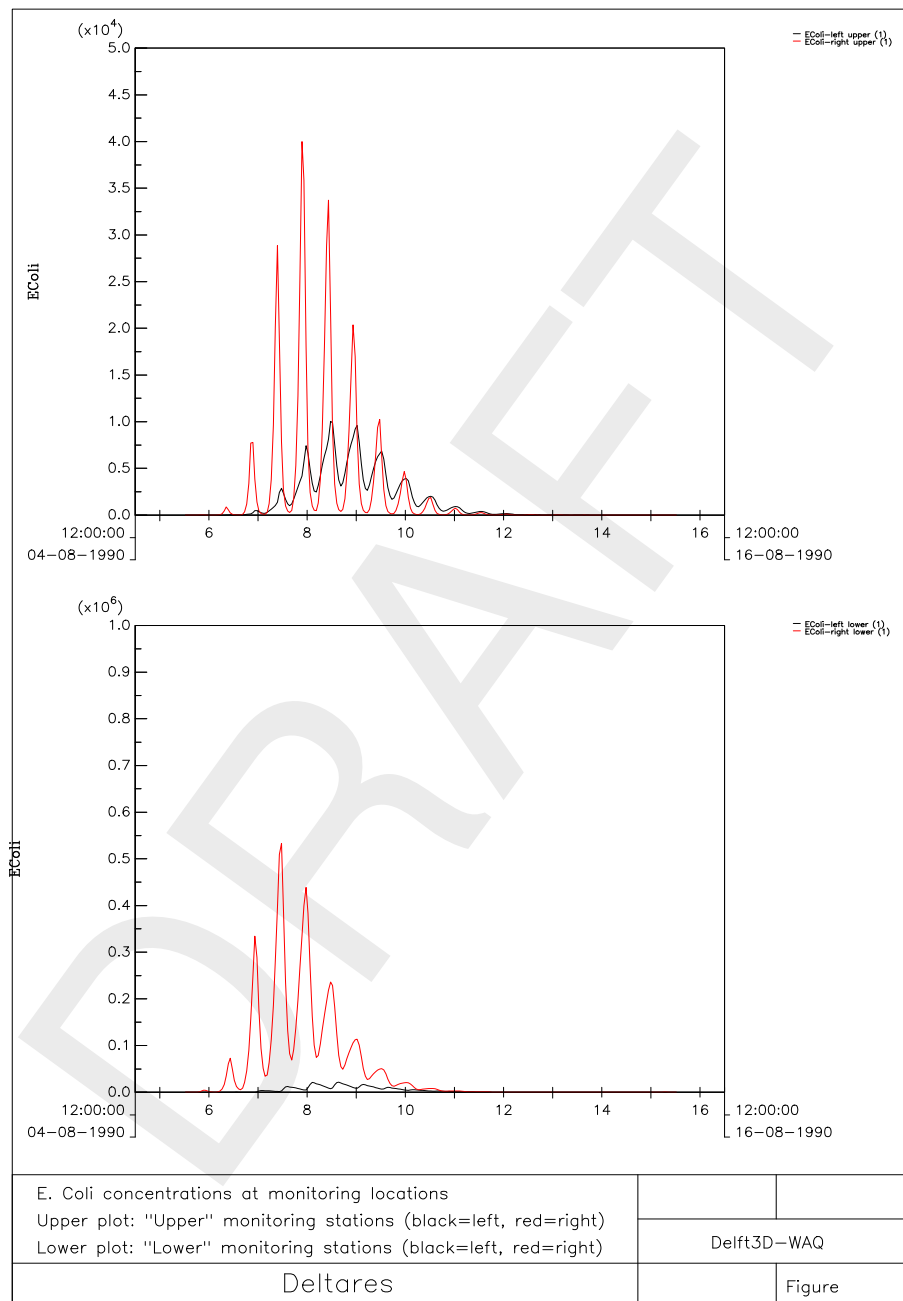


Figure 7.33: Time-series *E.Coli* concentration at monitoring stations (note the difference in scale); LEFT LOWER and LEFT UPPER (upper plot) and RIGHT LOWER and RIGHT UPPER (lower plot)

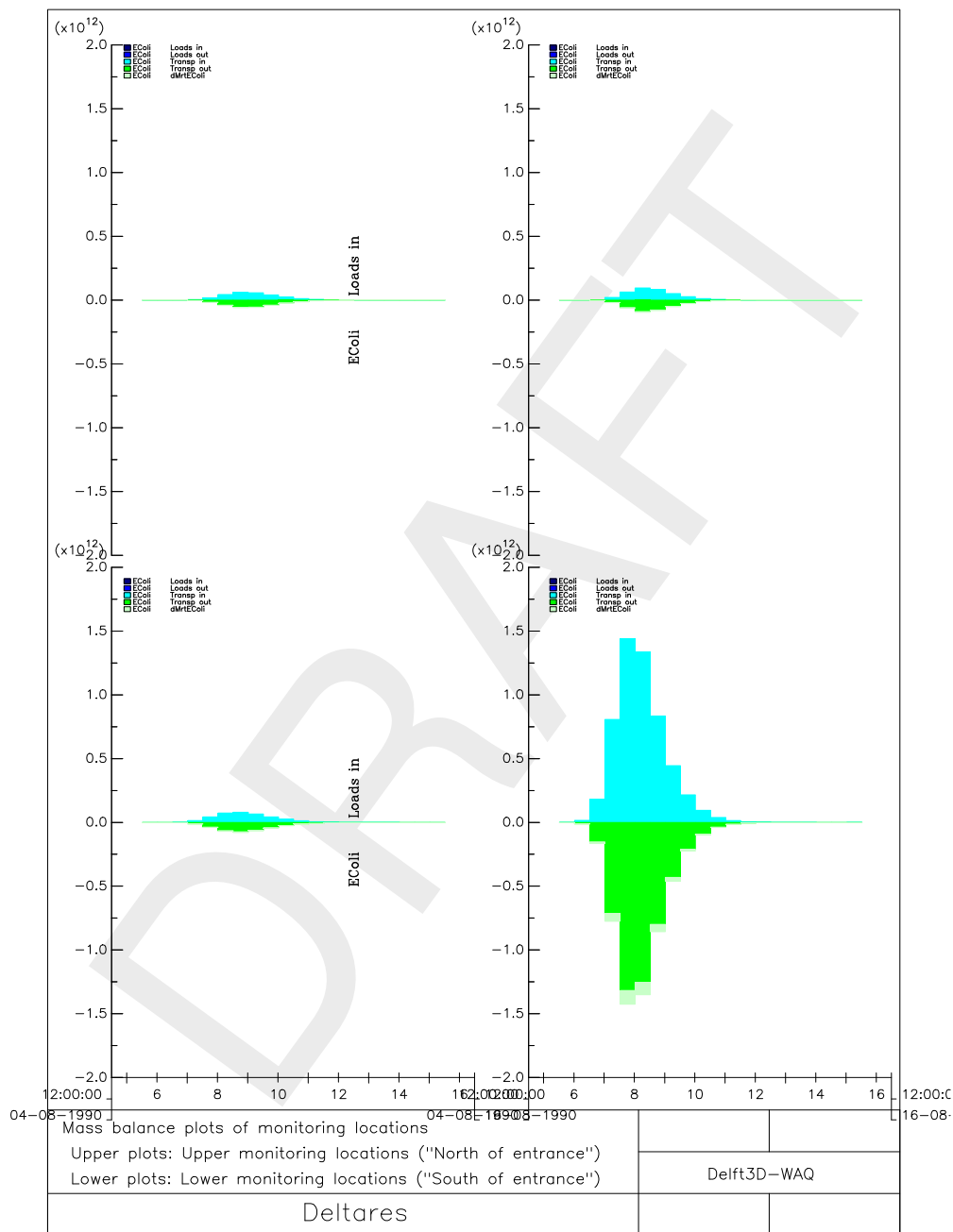


Figure 7.34: Mass Balances E.Coli; upper plots: monitoring station north of tidal inlet, lower plots: stations south of inlet

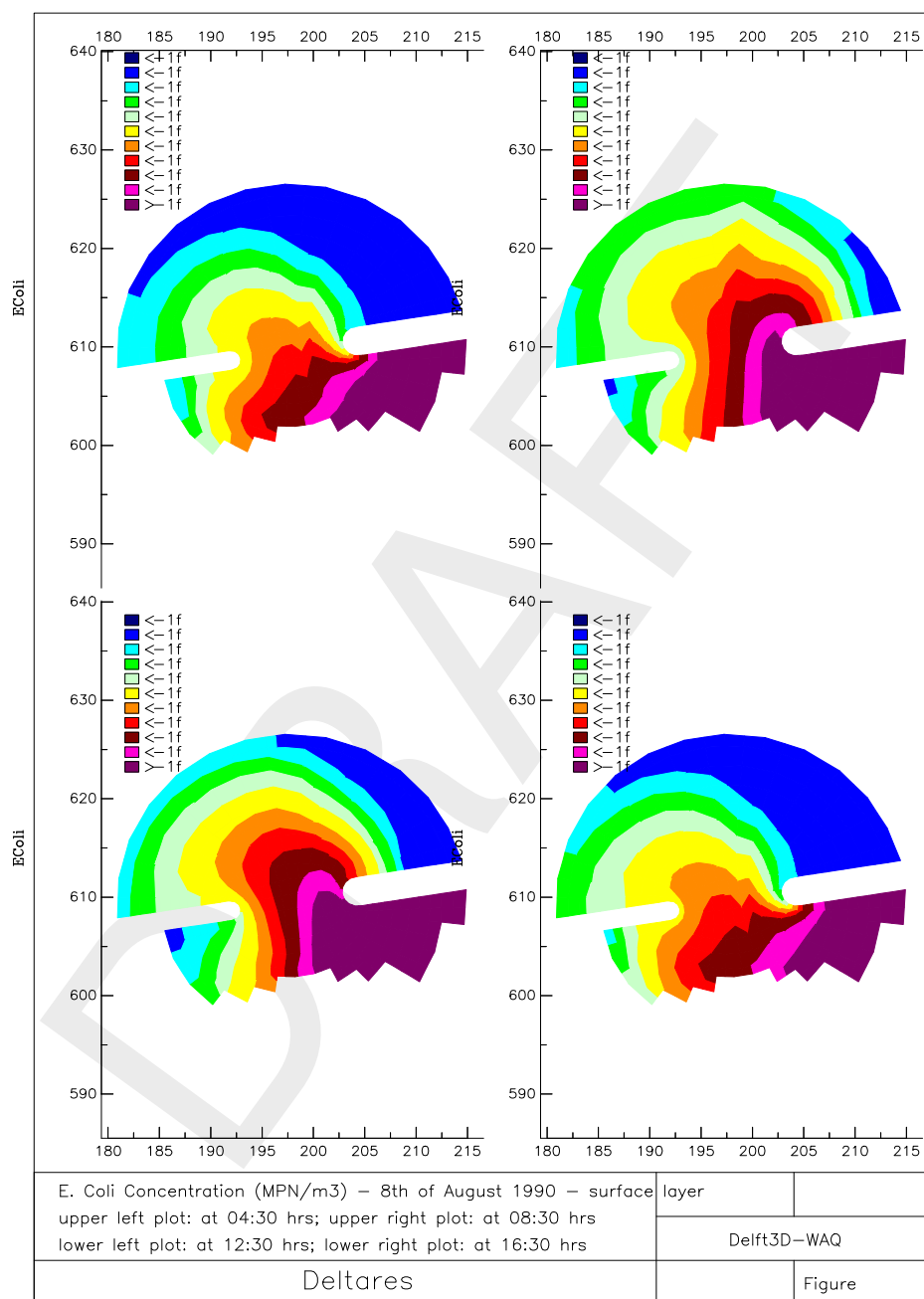


Figure 7.35: Contour plots of *E. coli* in the surface layer on 8 August 1990: 03:30 hr (upper left), 07:30 hr (upper right), 11:30 hr (lower left) and 15:30 hr (lower right)

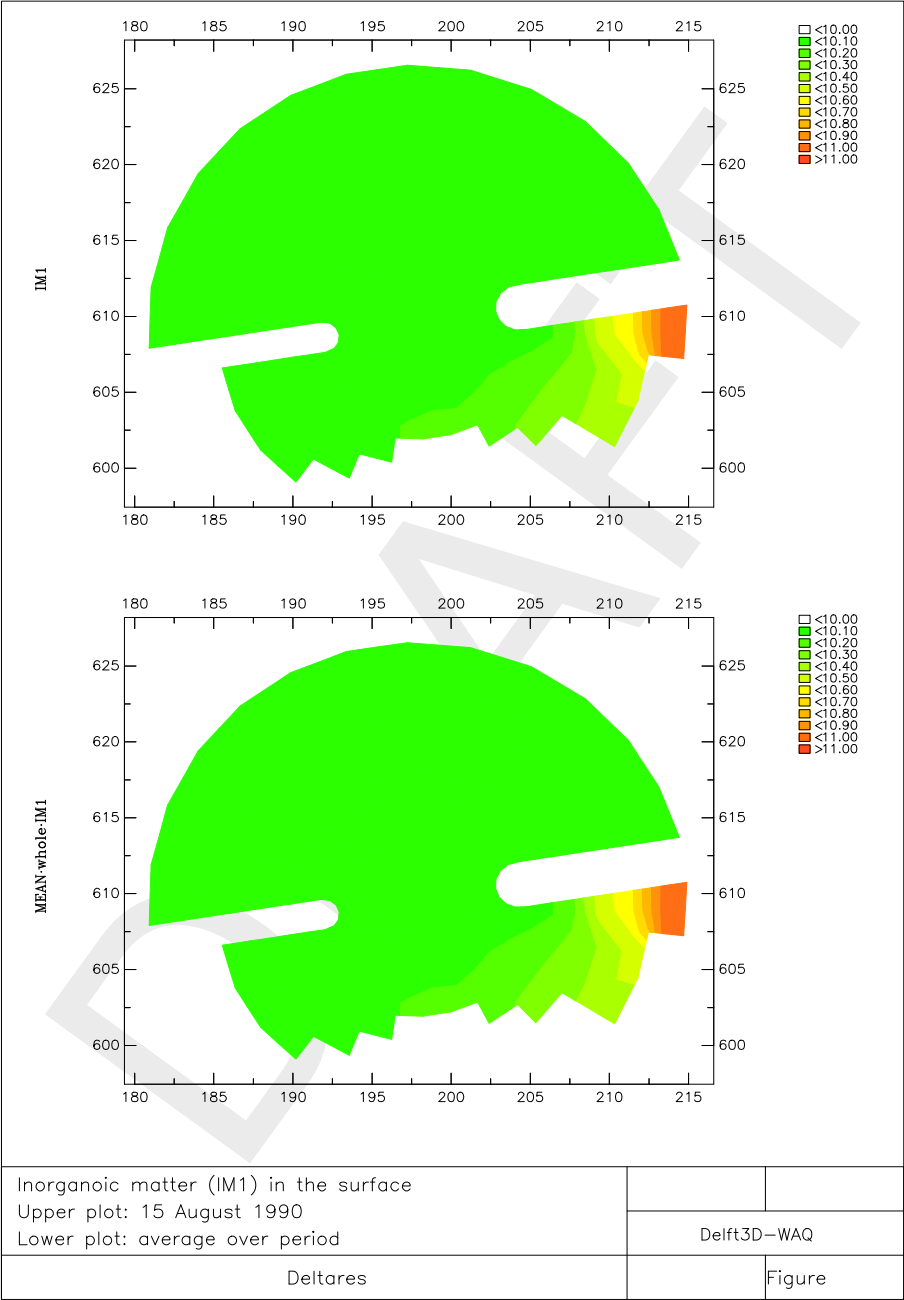


Figure 7.36: Inorganic matter concentration in the surface layer on 15 August 1990 12:30 hr (upper) and averaged over the simulation period (lower)

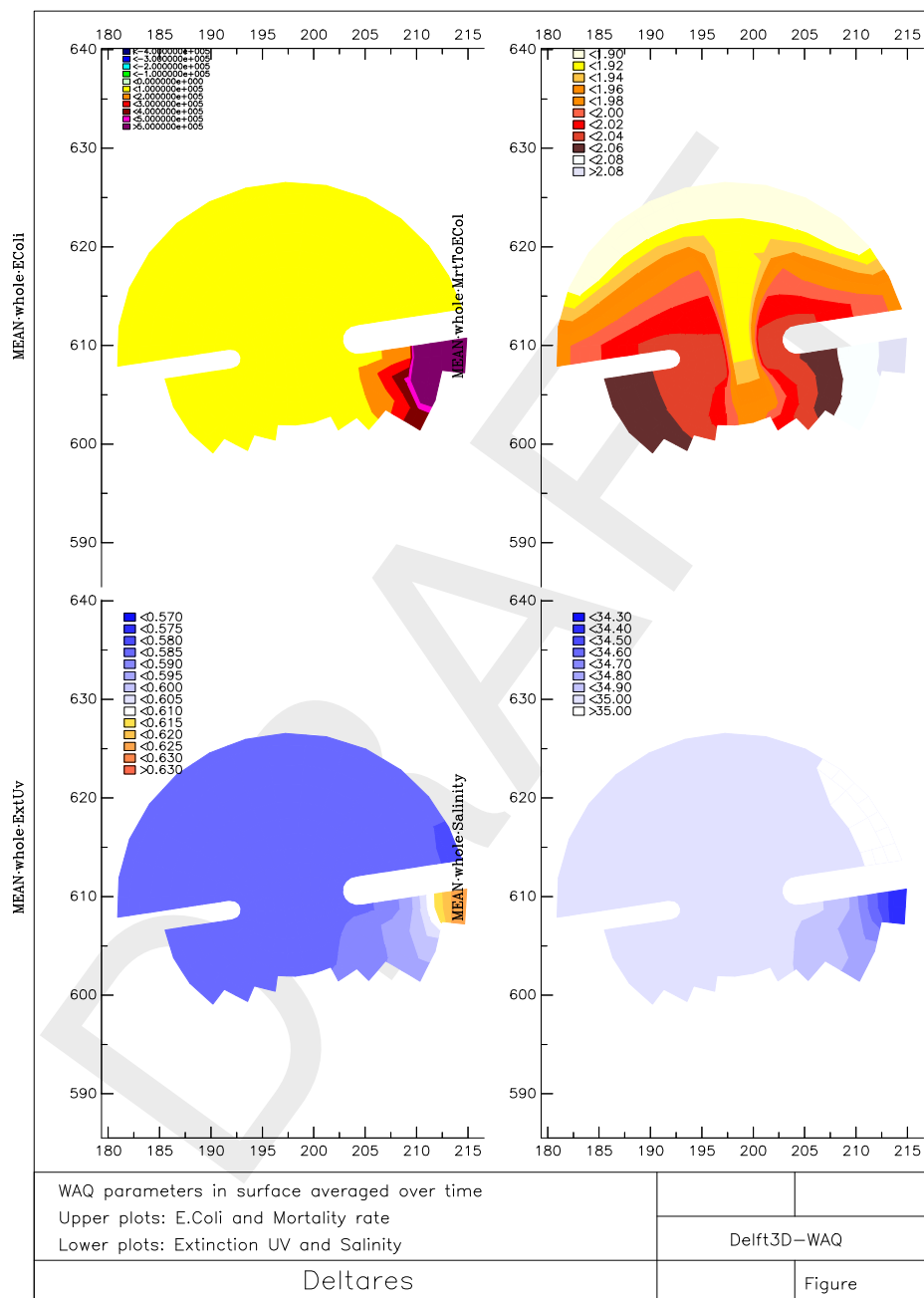


Figure 7.37: Water quality parameters in the surface layer averaged over time; *E.Coli* (upper left), extinction UV light (lower left), mortality rate (upper right) and salinity (lower left)

7.2 Tutorial Water Quality related to sewer overflows (SOBEK-Rural 1DWAQ + 1DFLOW modules)

7.2.1 How to set up a water quality model

This tutorial describes how to set up a water quality model with SOBEK-Rural 1DWAQ module. First a simple model will be set up, for an urban canal with one combined sewer overflow discharging to it. You will start from scratch and the tutorial guides you step by step through the schematisation and simulation processes. Once the model is finished you will use it to analyse the water quality problems related to combined sewer overflows. SOBEK-Rural 1DWAQ contains various options to present and analyse the simulation results. These techniques will be explained with help of the water quality model that you will set up.

7.2.1.1 Getting started

In this chapter a model will be set up for a single canal with one combined sewer overflow discharging to it. The schematisation of the water system will be combined with a water quality model for the simulation of oxygen and biochemical oxygen demand (BOD). At first the model will be used for the simulation of a period without any overflows.

- ◇ Click on the Windows *Start* button.
- ◇ Select the 'All Programs' or 'All Apps' menu.
- ◇ Select the 'Delft Hydraulics' menu.
- ◇ Select the 'SOBEK' menu item (SOBEK215).
- ◇ Click on the 'SOBEK' icon.
- ◇ Select the menu item 'Options' - 'SOBEK Options';
- ◇ Select the tab 'Background Map'.
- ◇ Select the file 'Tutorial1.map'.
- ◇ Press OK button to save and close SOBEK Options.
- ◇ Click the 'New Project' button.
- ◇ Type the name 'T_CSO'.
The program converts all the characters into upper case. If a project with the same name already exists, the user has to enter a different name here.
- ◇ Click the *OK* button.

You have added a new project with the name 'T_CSO'. You are now asked: do you want to work with this project?

- ◇ Click the *Yes* button.

The Case Manager appears, see below:

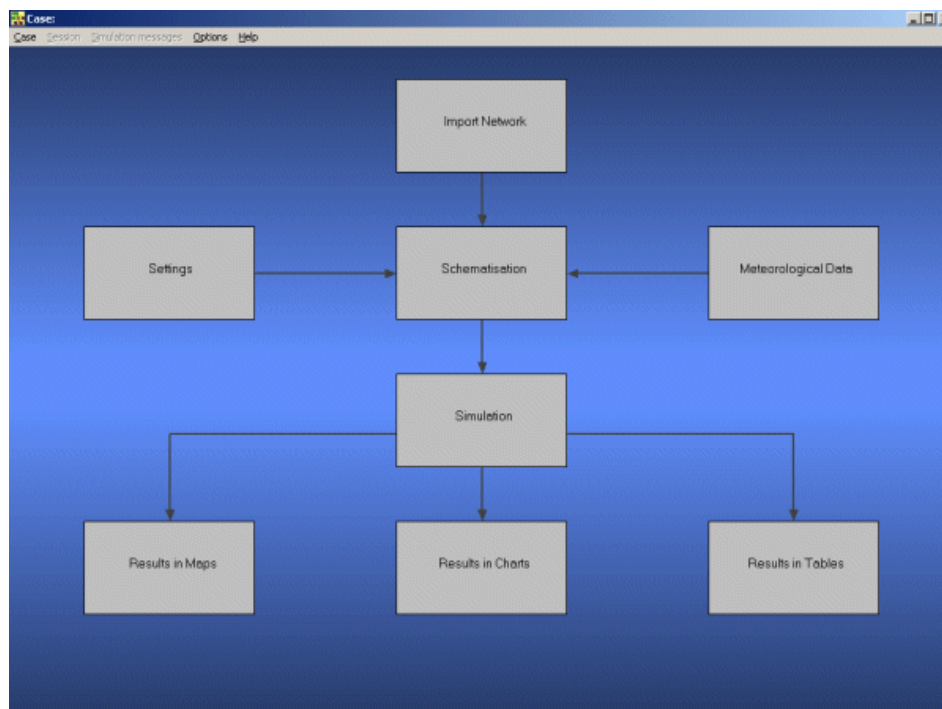


Figure 7.38: The case manager window.

- ◇ Select the menu 'Case' - 'Open as new'.
- ◇ Enter the name "Reference model".
- ◇ Click the *OK* button.

In the Case Manager, the task block Settings, Import Network and Meteorological Data are yellow, the other task blocks are red. The colour of the task block indicates the actions that the modeller still has to perform. Yellow indicates that in this task block still some work has to be done, before one can continue with the red task blocks. Once a task is finished, the colour of the task block turns into green.

7.2.1.2 Task block: Import network

- ◇ Double click the task block 'Import Network' in the case manager.
- ◇ Choose 'Start from scratch'.
- ◇ Click the *OK* button in order to leave the task block 'Import Network' and return to the Case Manager.

7.2.1.3 Task block: Settings

- ◇ Double click the task block 'Settings' in the Case Manager.
- ◇ Unselect all the selected modules if any.
- ◇ Select the module '1DFLOW (Rural)'.
- ◇ Select the module '1DWAQ'.
- ◇ Click the *OK* button (The output of the 1DFLOW module(s) is set to mean values!).

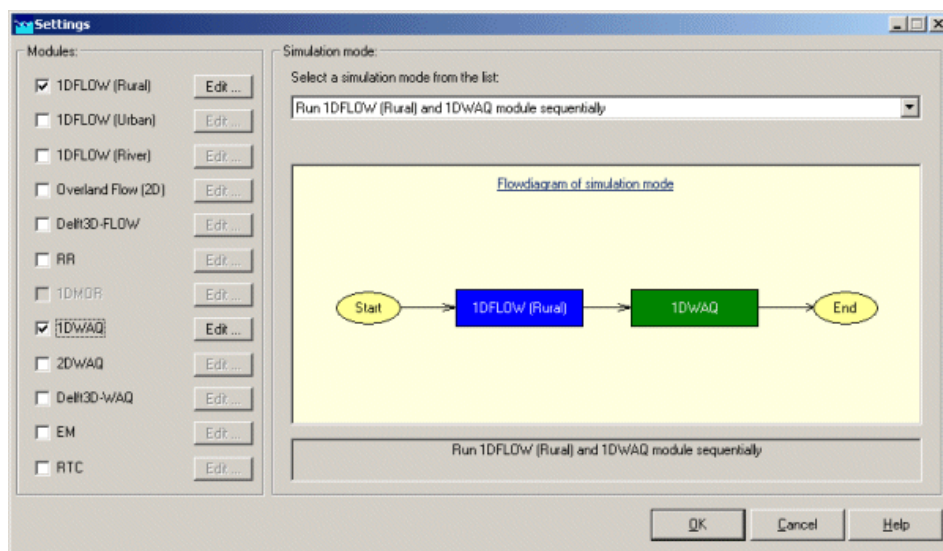


Figure 7.39: The Settings window.

- ◇ Click the *Edit...* button of the '1DFLOW (Rural)' module.

The tab with 'Time settings' appears.

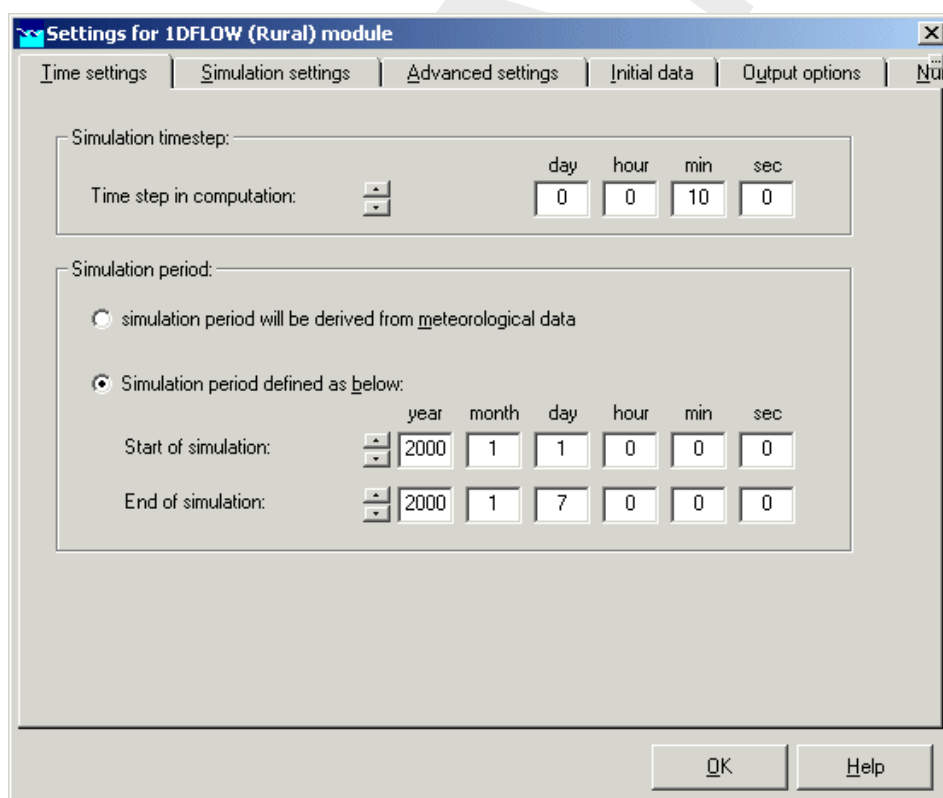


Figure 7.40: The tab with the time settings for the hydraulic calculation: simulation period and the time step for calculation.

- ◇ Make the 'Time step for computation' 10 minutes.
- ◇ Select the option 'Simulation period defined as below'.
- ◇ Change the simulation period, it starts on 1st of January, 2000 00:00:00 and ends on the 7th of January, 2000 00:00:00.

- ◇ Go to the tab 'Simulation settings'.
- ◇ In the group box 'Simulation mode:', select 'unsteady calculation'.
- ◇ Go to the tab 'Initial data'.
- ◇ Choose the option 'define global initial values'.
- ◇ Select the option 'initial depth in channels [m]'.
- ◇ Enter an initial water depth of "0.5" m.
- ◇ Go to the tab 'Output options'.
- ◇ Select a 'Time step output' of '10 minutes'.
- ◇ The default 'output parameters' are correct for this simulation.
- ◇ Click the *OK* button.

A message appears about the time step of the 1DWAQ module and the output time step of the 1DFLOW module.

- ◇ Click the *OK* button.
- ◇ Click the *OK* button.
- ◇ Click the *Edit* button of the '1DWAQ' module in the Settings window.

The tab with 'Time step settings' appears.

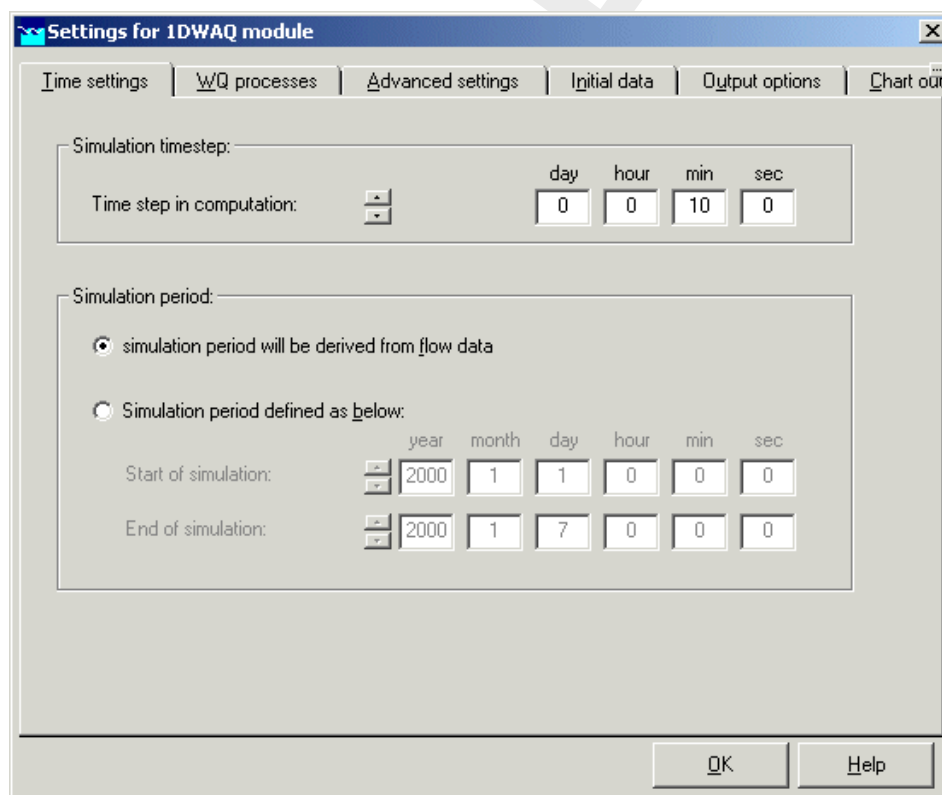


Figure 7.41: The tab for the adjustment of the time step in the computation and the simulation period of the water quality simulation.

- ◇ Adjust the 'Time step in computation' to 10 minutes.
- ◇ Select the option 'Simulation period will be derived from flow data'.
- ◇ Go to the tab 'WQ processes'.
- ◇ Select 'Calculate water quality transport'.

Now the transport of substances is activated.

- ◇ Select 'active processes'.

Now the water quality processes that act on the substances are activated.

- ◇ Go to 'Advanced settings';

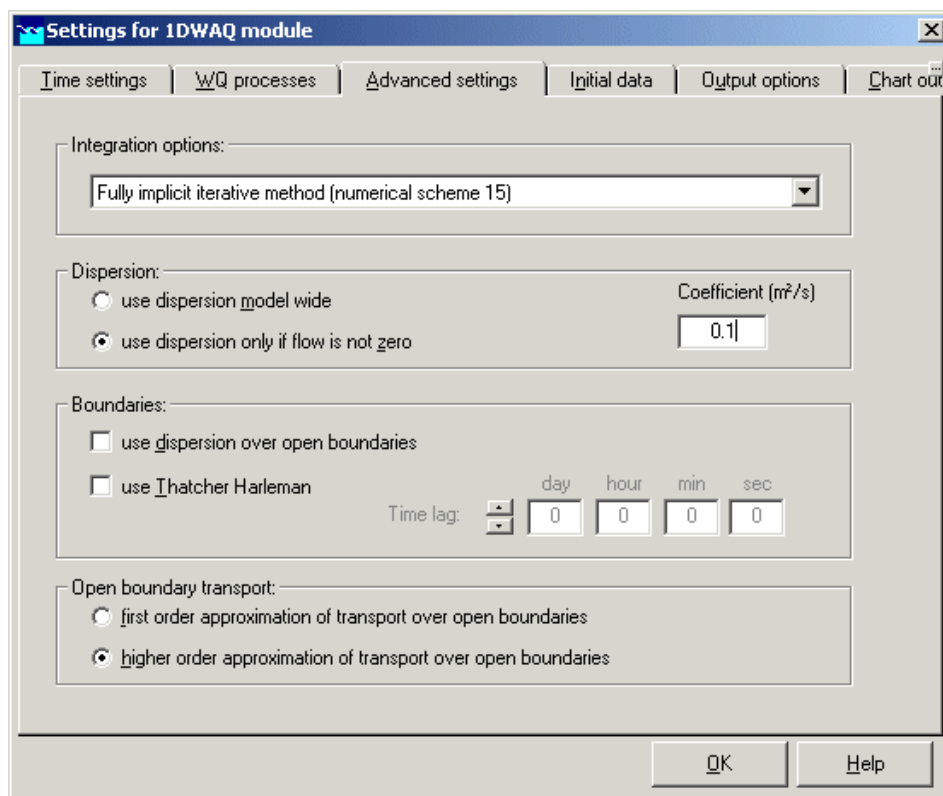


Figure 7.42: The tab where the numerical solver can be selected and some dispersion parameters can be adjusted.

On this tab one can choose a numerical solver from an extended list of different schemes. These solvers differ from each other in the amount of numerical dispersion that occurs during the simulation. The selected solver also determines the time that a computation takes. With some solvers the computing time of a simulation is significantly higher. For instance for urban canal networks with a number of interconnections, the 'Fully implicit iterative scheme' is the preferred solver. A realistic dispersion coefficient for small, urban water system with low flow velocities is in the range of $0.1 \text{ m}^2/\text{s}$ to $0.5 \text{ m}^2/\text{s}$.

- ◇ Choose for the 'Fully implicit iterative method' (Numerical scheme 15) from the 'Integration options'.
- ◇ Choose 'Use dispersion only if flow is not zero'. The dispersion will be taken into account only if the flow velocity is not zero.
- ◇ Enter a dispersion coefficient of " $0.1 \text{ m}^2/\text{s}$ ".

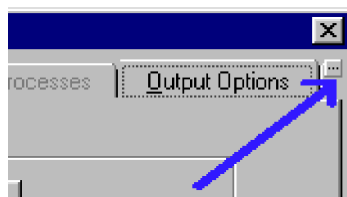


Figure 7.43: Click this button to unveil the tabs "chart output" and "map output"

- ◇ Go to the tab 'Chart Output'.
- ◇ Enter "30" minutes.
- ◇ Go to the tab 'Map Output'.
- ◇ Enter "30" minutes.

7.2.1.4 The predefined subset

On the tab 'WQ Processes' the set of processes that are active in the water quality model can be composed. It is also possible to choose from a number of pre-defined subsets of water quality processes. In this tutorial a 'predefined subset' of water quality processes will be used.

There are three pre-defined subsets available for the simulation of water quality in urban surface waters:

- ◇ Tewor+ model for SOBEK (Oxygen).
- ◇ Tewor+ model for SOBEK (Oxygen and nutrients).
- ◇ Tewor+ model for SOBEK (Complete).

The subsets are based on the Dutch TEWOR+ model. [Table 7.12](#) summarises the substance groups in each pre-defined subset.

Table 7.12: Overview of substance used for TEWOR

| Subset: Substance groups: | Tewor+Oxygen | Tewor+Oxygen, Nutrients | Tewor+Complete |
|------------------------------|--------------|----------------------------|----------------|
| Oxygen and BOD | ✓ | ✓ | ✓ |
| Nitrogen | ✓ | ✓ | ✓ |
| Phosphorus | | ✓ | ✓ |
| Suspended Solids | | ✓ | ✓ |
| Bacteria | | | ✓ |
| Heavy Metals | | | ✓ |
| Organic Micro pollutants | | | ✓ |
| Chloride | | | ✓ |

In this tutorial you will use the pre-defined subset *Tewor+ model for SOBEK (Oxygen)*.

- ◇ Go to the tab *WQ Processes*.

- ◇ Choose for the option *use predefined process*.
- ◇ Select the pre-defined subset *Tewor+ model for Sobek (Oxygen)*.

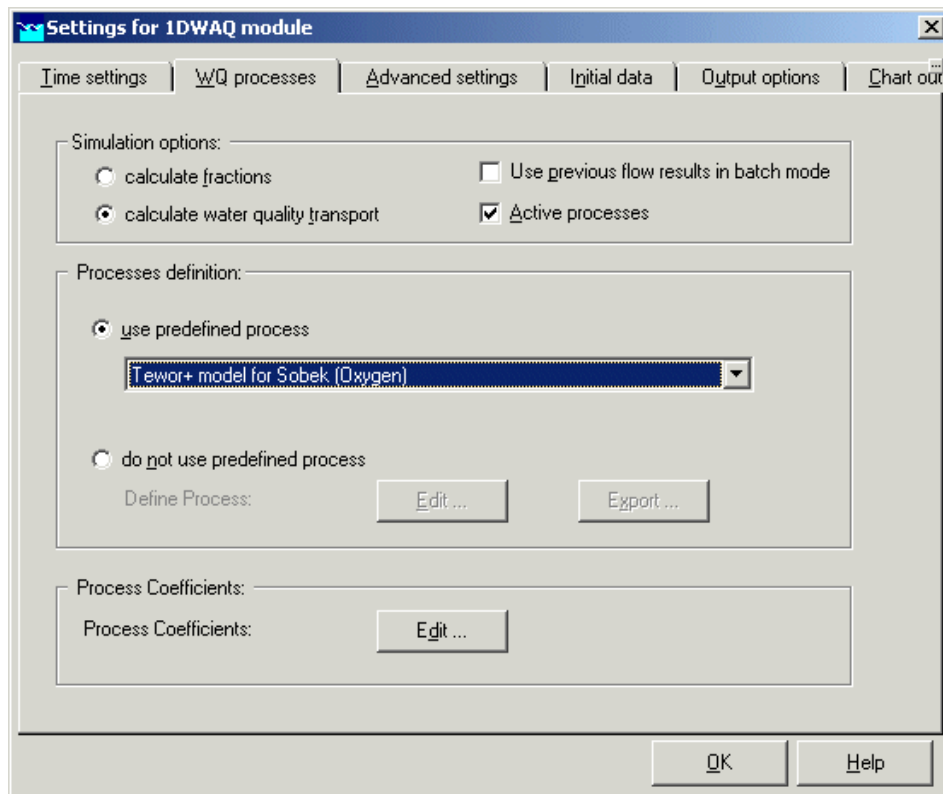


Figure 7.44: Selecting a predefined subset.

7.2.1.5 Process coefficients

- ◇ Click the *Edit...* button next to 'Process Coefficients'.

In the table that is shown in [Figure 7.45](#), the process coefficients can be entered. Before the model is calibrated (the calibration is described further in this tutorial), default parameter values are used.

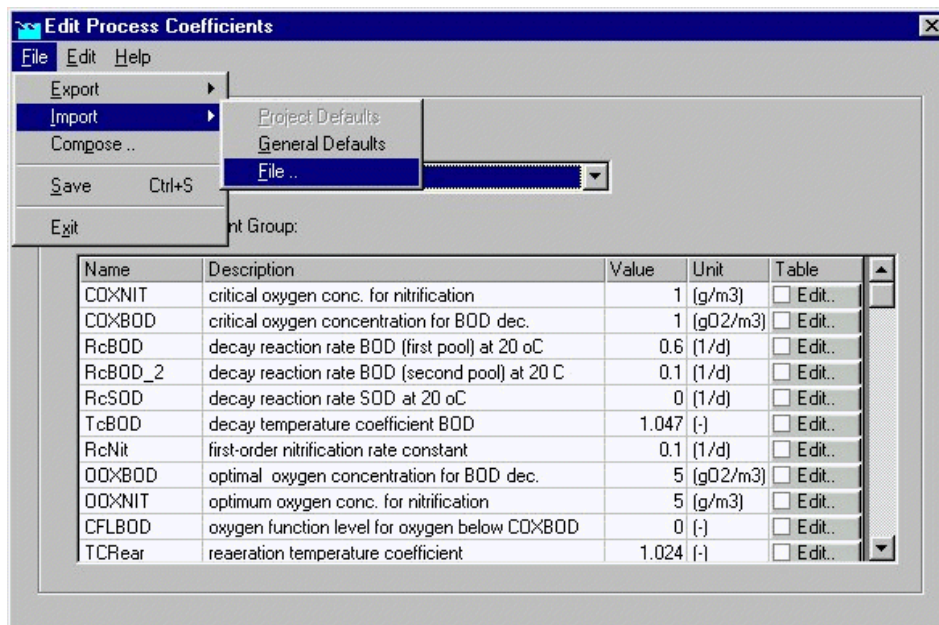


Figure 7.45: The table of process coefficients.

- ◇ Set the parameters to default values in the menu 'File' - 'Import' - 'File'.
- ◇ Select the file 'Tewor+_oxygen.plc' in the directory '\SOBEK215\Fixed\Delwaq\'.
 ◇ Press the *Open* button.
- ◇ Save the parameters via the menu 'File' - 'Save'.
- ◇ Leave the table with process coefficients via 'File' - 'Exit'.

A warning appears, saying that you should also enter the initial values. We will do that in the following chapter.

- ◇ Press the *OK* button.

7.2.1.6 Initial conditions

- ◇ Go to the tab 'Initial data'.
- ◇ Click the *Edit* button next to 'use global initial values'. In the table the initial values can be entered.

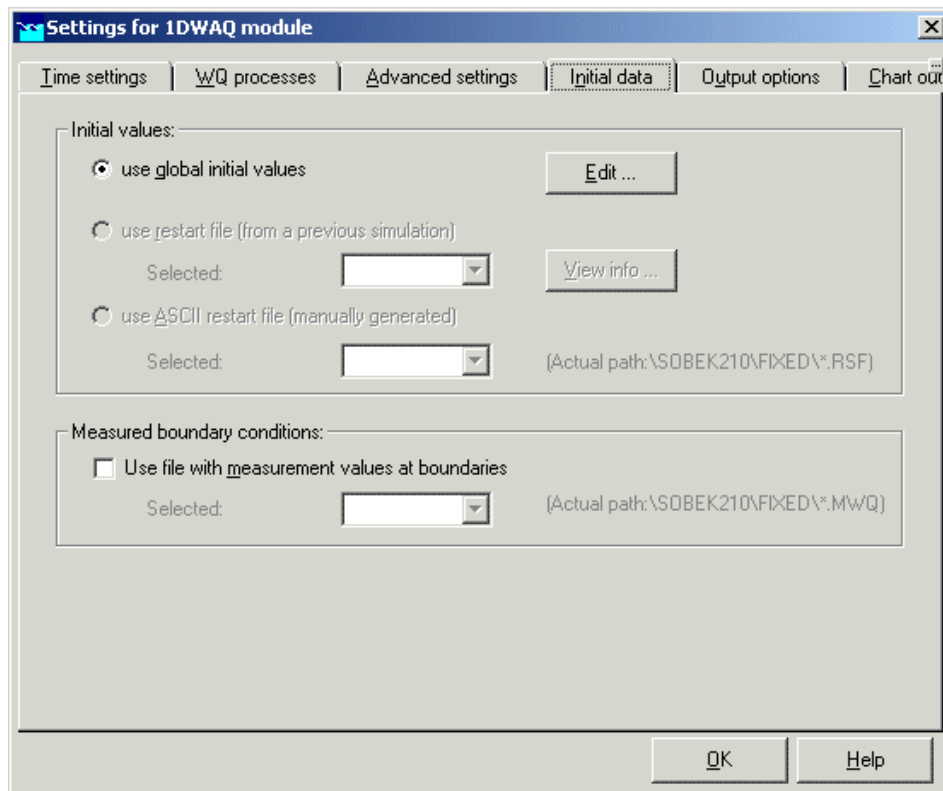


Figure 7.46: The Initial data tab.

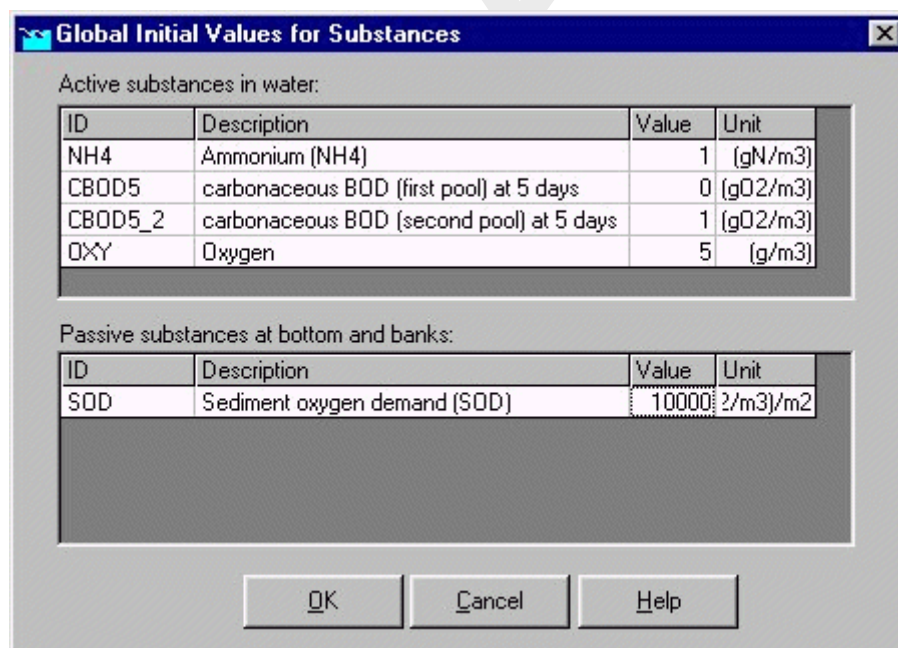


Figure 7.47: Global Initial Values for Substances.

- ◇ Enter the values as depicted in [Figure 7.47](#).
- ◇ Click *OK* to leave the input screen for initial conditions.
- ◇ Click *OK* to leave the 1DWAQ Settings.
- ◇ Click *OK* to leave Settings and return to the Case Manager.

7.2.1.7 Meteorology

SOBEK-Rural simulations require meteorological input data, i.e. precipitation data, evaporation data, wind data, water temperature and solar radiation. The Meteorological data task block provides precipitation and evaporation data to the RR (Rainfall-Runoff) module, wind data to the 1DFLOW and Overland Flow (2D) modules and water temperature and solar radiation data to the 1DWAQ and 2DWAQ modules. For simplified rainfall-runoff processes precipitation data can optionally be provided to the 1DFLOW and Overland Flow (2D) modules.

- ◇ Double-click the 'Meteorological Data' task block of the Case Manager.

The following screen will appear:

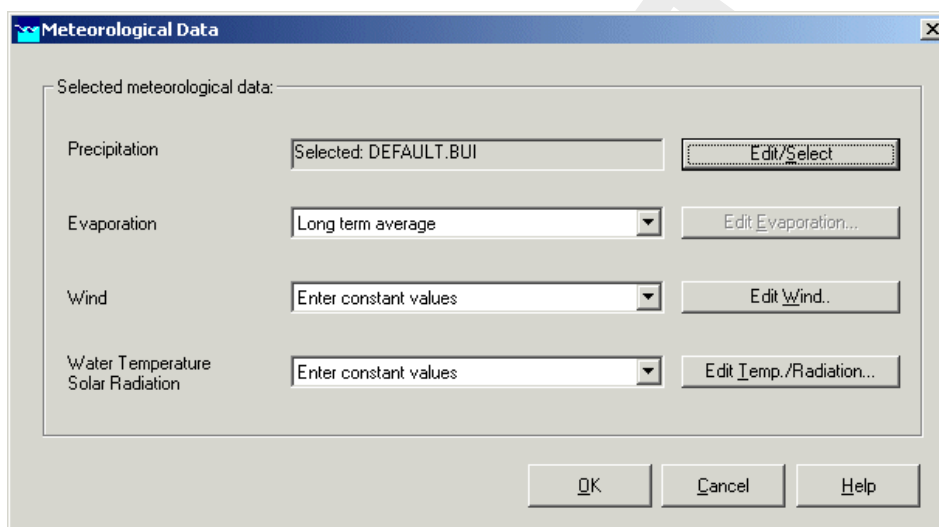


Figure 7.48: The *Meteorological Data* window.

In the dialog that pops up you can see how precipitation, evaporation, wind, water temperature and solar radiation data are defined.

- ◇ Click the *Edit Wind...* button.
- ◇ Set the wind velocity to 0 m/s.
- ◇ Press the *OK* button.
- ◇ Click the *Edit Temp./Radiation...* button.
- ◇ Enter a water temperature of "18.2" °C.
- ◇ Enter a 'Solar Radiation' of "50" W/m².
- ◇ Press the *OK* button.
- ◇ Click *OK* to leave the task block 'Meteorological Data' and to return to the Case Manager.

Now you have finished defining the meteorological data. Notice that this task block has turned green too!

7.2.1.8 Task block: Schematisation

- ◇ Double click the task block 'Schematisation'.

The window below appears:

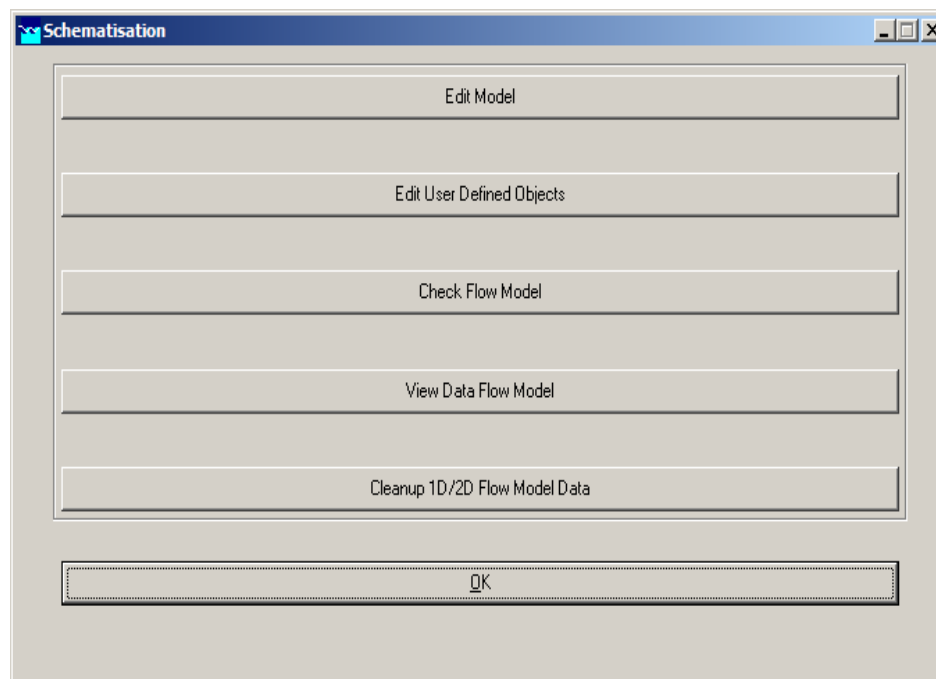


Figure 7.49: The **Schematisation** window.

- ◇ Click the *Edit model* button.

When the option *Edit Model* of the 'Schematisation' is selected, the network editor starts.

The network editor is called NETTER and is a component of the Delft Hydraulics Decision Support System (Delft-DSS) tools. NETTER offers the possibility to set-up the schematisation on top of a background GIS map. NETTER also offers advanced analysis tools to show model results linked to the schematisation and provide the user with full printing facilities to make high quality prints.

Within NETTER you can do the following:

- 1 Interactively and graphically prepare a schematisation;
- 2 Generate schematisations upon GIS map Layers;
- 3 Carry out schematisation operations: search for a certain node, show node numbers and names, show link numbers, etc.;
- 4 Carry out map operations: zooming in, zooming out, (de)activating map layers, colouring of map layers, adding title information on the map, etc.;
- 5 View results of simulation models for schematisations created in NETTER;
- 6 Print maps or schematisations on one or more pages which fit together.

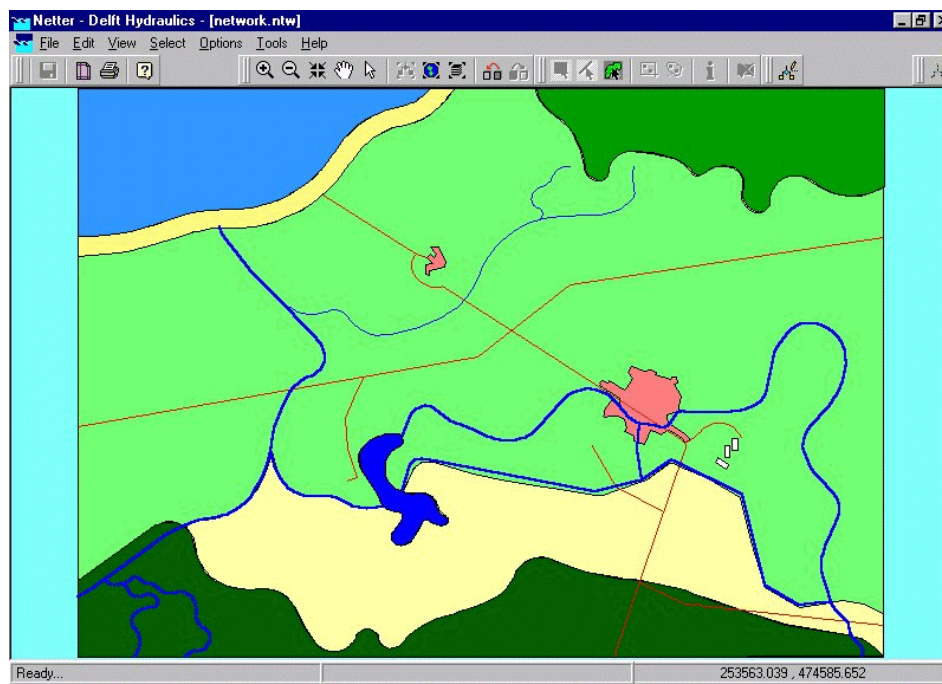




Figure 7.50: The hypothetical town (SOBEK CITY)


In order to focus on a small part of the map, you can use the zoom functionalities.

The View menu contains commands to zoom in, zoom out, centre the window, move the window and show all schematisation or map layers.


The  button allows you to zoom in on any part of the "active main window".


The  button allows you to zoom out by shrinking the displayed part of the "active main window".


The  button allows you to centre a schematisation or map GIS object. When choosing this command and then clicking with the left mouse button on an object NETTER, redraws the map centring the chosen object to the NETTER window.


The  button allows you to shift the view by clicking the mouse anywhere in the NETTER window and dragging the view to another position.

The  button redraws the view fitting all schematisation objects into the NETTER window.

The  button redraws the view fitting all GIS map layers into the NETTER window.


The  button restores the view of the map before the last zoom command was given.

The  button restores the view of the map before the last 'Show Previous' command was given.

- ◇ Use the  button to zoom in on the town and the river.

7.2.1.9 Working with NETTER

Six bars with buttons are available for making schematisations: 'Node', 'Connection', 'Reach', 'Flow model', 'Edit Network' en 'Edit Reach Vectors'. The button bars are separate windows that can be dragged to a convenient place on the screen. In this way you can customise NETTER.

- ◇ Go to the menu 'Edit' and subsequently 'Network'.
- ◇ Click  button next to the button 'No edit action' in the 'Edit network' menu.

A list with menu-options appears:

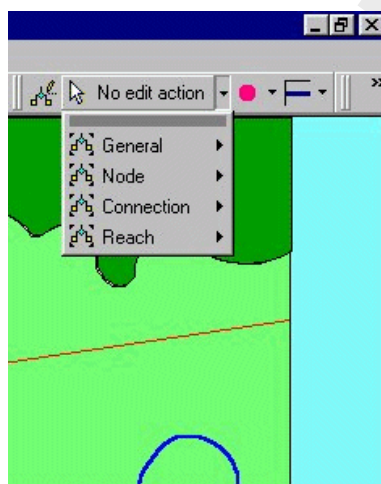


Figure 7.51: The menu Edit Network.

- ◇ Move the mouse to 'Node'.

A window with buttons rolls down, as shown below.

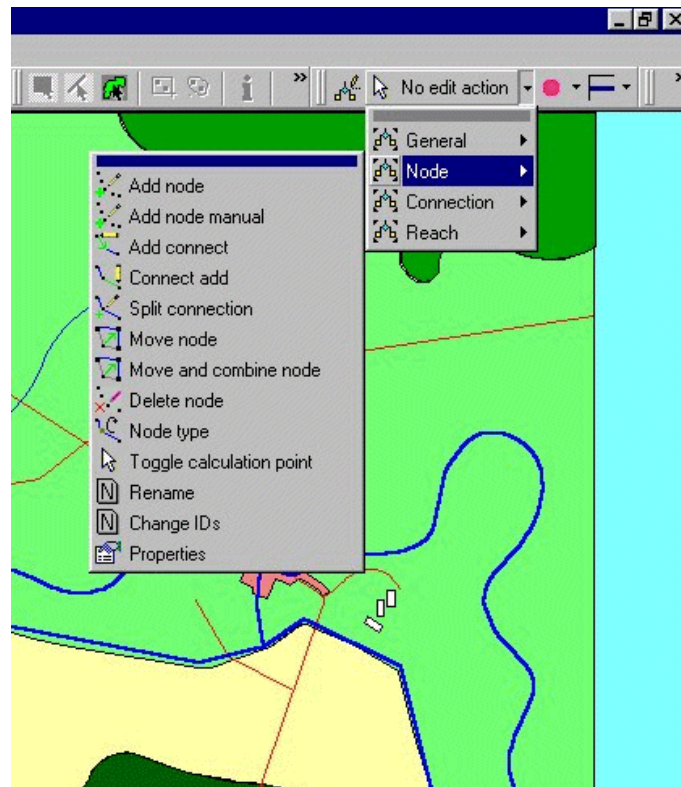


Figure 7.52: The menu Node.

- ◇ Keep the mouse on the coloured bar;
- ◇ Keep the left mouse button pressed and drag the button bar 'Node' over the window;
- ◇ Do the same for the button bar 'Connection';
- ◇ Do the same for the button bar 'Reach'.
- ◇ Do the same for the button bar 'Flow model'.

An example of NETTER, with all button bars visible is shown below.

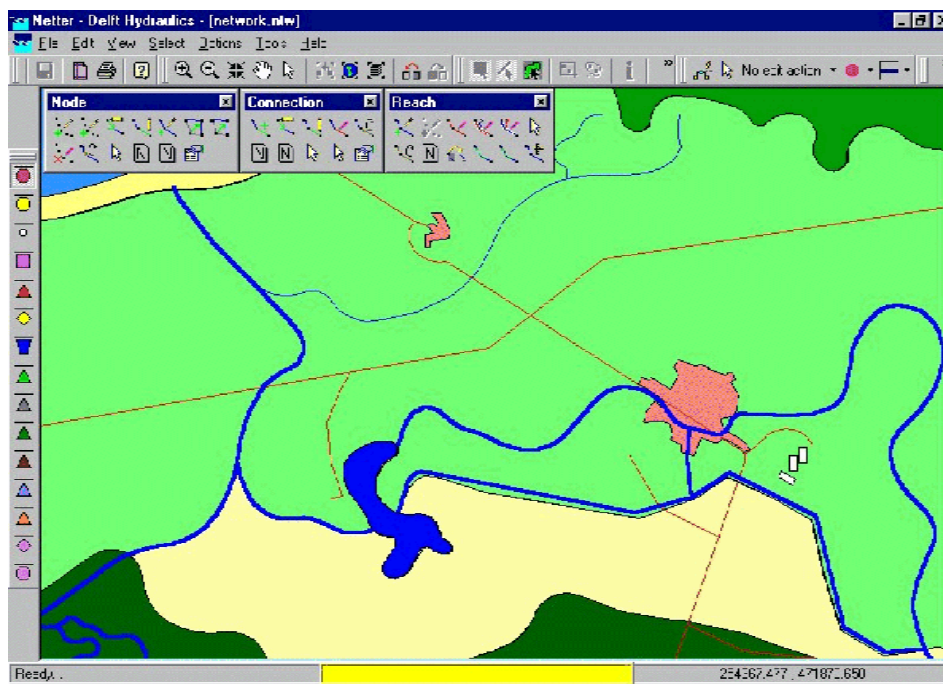



Figure 7.53: The button bars in NETTER.

7.2.1.10 The schematisation



In this paragraph we are going to make a simple schematisation of a small river, to which one combined sewer overflow is discharging.

The boundaries of the model are: a constant discharge (east) and a fixed water level (west). The sewer overflow is modelled as a lateral discharge.

All model components need to have unique identifiers. It is possible to define the identifiers (or IDs) of the nodes and branches (links) automatically or manually.

- ◇ Select the  button in the 'General' tool bar, Edit settings, to go to the edit network options.
- ◇ Select the tab 'Node'.
- ◇ In the 'ID' group box, select the radio button 'Manual'.
- ◇ In the 'Name' group box, select the radio button 'Manual'.
- ◇ Select the tab 'Link'.
- ◇ Set the 'ID' and 'Name' to 'automatic'.
- ◇ Click the *OK* button.

During this tutorial we will build a small network as shown in [Figure 7.56](#).



- ◇ Click the object 'Flow - boundary' in the menu Flow-model: .
- ◇ Click the button 'Add node' of the menu 'Node': .
- ◇ Enter "Inflow" in both input fields.
- ◇ Press the *OK* button.
- ◇ Place the boundary node east of the town, by clicking on the map with the left mouse button.




Remark:

- ◇ Although it is possible to work with object IDs of more than 20 characters in the D-Flow 1D modules, D-WAQ 1D can only work with IDs of 20 characters or less. Because IDs can be prefixed with an 'n' when using D-WAQ 1D, any network objects used during a D-WAQ 1D simulation should have a maximum ID length of 19 characters.

In order to see the identifiers on the map please:



- ◇ Click on the  button in the Active Legend or select the menu item 'Options' - 'Network Data...'.
 - ◇ Select the tab 'Node'.
 - ◇ Select the radio button 'Name'.
 - ◇ Press the *OK* button.
- ◇ Click the button 'Add node' of the menu 'Node': .
 - ◇ Enter "Outflow" in both input fields.
 - ◇ Press the *OK* button.
 - ◇ Place a boundary node west of the town, by clicking on the map with the left mouse button.

The river flows from east to west through the town.

- ◇ Click the button 'Connect nodes' of the menu 'Connection': .
 - ◇ Connect the two buttons by clicking with the left mouse button on the node 'Inflow' in the east and dragging with the left mouse button pressed from the node 'Inflow' in the east to the node 'Outflow' in the west.

The simulation will be more accurate if a calculation grid is used, for instance with a distance of 50 m between the nodes. Another advantage is the fact that this will make output available on more locations.

But before we will generate a calculation grid we will change the general edit settings.

- ◇ Select the  button in the 'General' tool bar, Edit settings, to go to the edit network options.
 - ◇ Select the tab 'Node'.
 - ◇ In the 'ID' group box, select the radio button 'Automatic'.
 - ◇ In the 'Name' group box, select the radio button 'No Names'.
 - ◇ Click the *OK* button.
- ◇ Click the button 'calculation grid all reaches' of the menu 'Reach': .
 - ◇ Select the 'Split vector' option in the 'Calculation points' window.
 - ◇ Enter value "50" for length.
 - ◇ Select 'Equidistance'.
 - ◇ Then press the *OK* button.

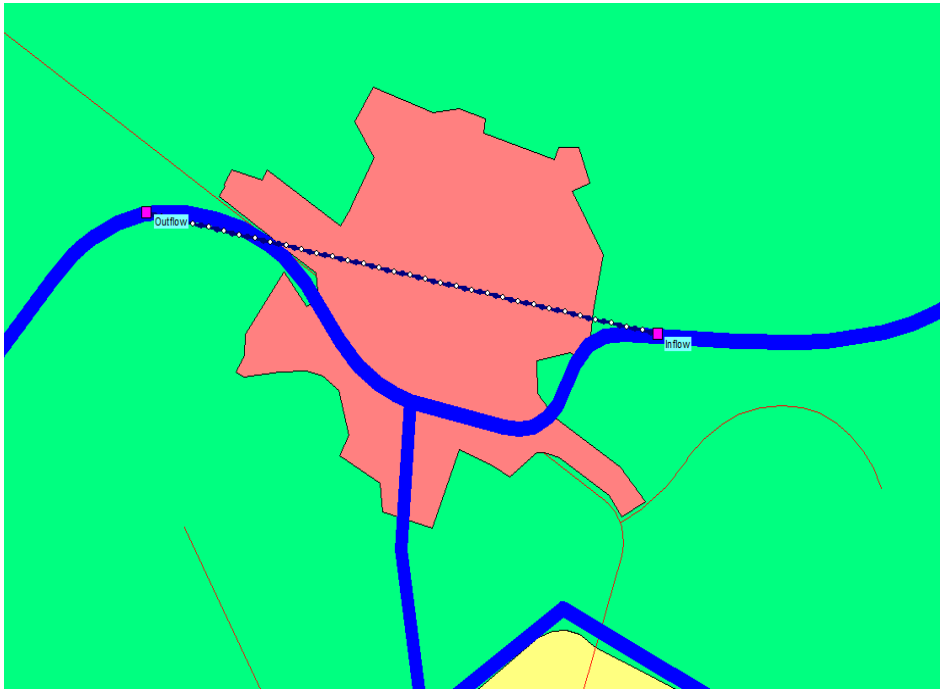


Figure 7.54: The (provisional) model schematisation in NETTER.

The schematisation is still a straight line crossing town. But we would like to see that the schematisation follows the river as closely as possible.

- ◇ Go to the menu 'Edit' and subsequently 'Vector Layer'.

The menu 'Edit reach vectors' appears.

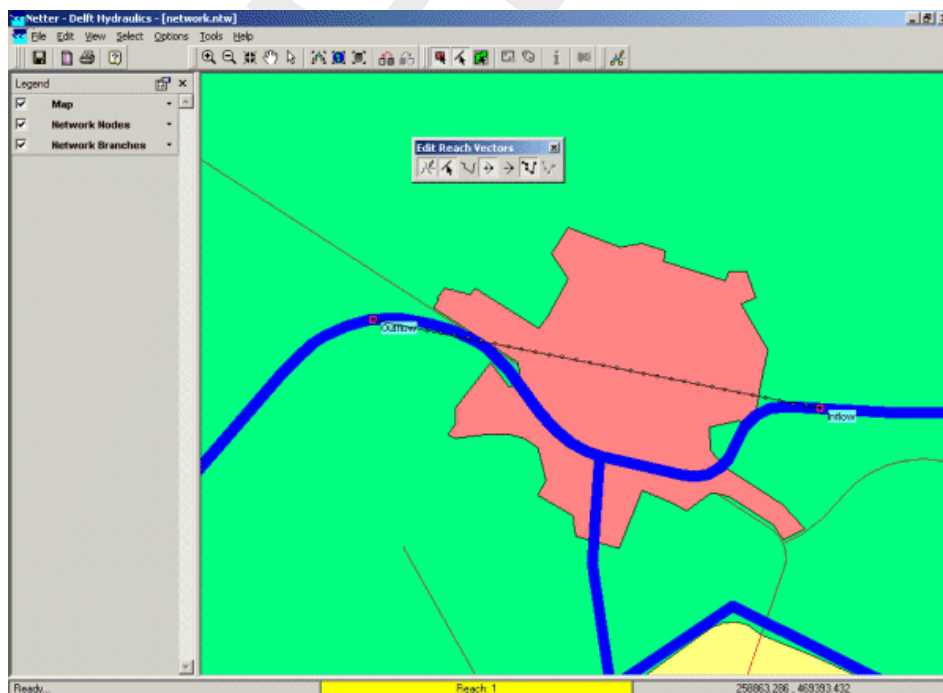





Figure 7.55: The menu 'Edit reach vectors'.

The reach is shown as a thin black line now. If you point to the reach, the cursor has the form a thin black arrow.

- ◇ Click the button 'Show co-ordinates': .
- ◇ Click the reach in order to select it.
- ◇ Click the button 'Add co-ordinate' of the menu 'Edit reach vectors': .
- ◇ Click with the left mouse button on the reach and drag the coordinate to its new location.
- ◇ Grab the reach with the cursor by repeating the last step at several places and bend the reach towards the river.
- ◇ Click the button 'Edit reach vectors':  and the network will be fixed in this position.




In the following steps we will add a sewer overflow and two cross section profiles as shown in Figure 7.56.



Figure 7.56: The completed 1DWAQ tutorial schematization.




The sewer overflow is modelled as a lateral discharge to the river.

But before we will add the 'Flow - Lateral Flow' node we will change the general edit settings.

- ◇ Select the  button in the 'General' tool bar, Edit settings, to go to the edit network options.
- ◇ Select the tab 'Node'.
- ◇ In the 'ID' group box, select the radio button 'Manual'.
- ◇ In the 'Name' group box, select the radio button 'Manual'.
- ◇ Click the OK button.
- ◇ Click the object 'Flow - Lateral Flow' of the menu 'Flow model': .
- ◇ Click the button 'Add node' of the menu 'Node': .
- ◇ Enter "CSO" in both input fields.

- ◇ Press the *OK* button.
- ◇ Add the sewer overflow to the network by clicking with the left mouse button on the reach.

The river has two known cross section profiles. It is assumed that between these the profiles can be calculated by interpolation.

- ◇ Click the object 'Flow - Cross section' of the menu 'Flow model': .
- ◇ Click the button 'Add node' of the menu 'Node': .
- ◇ Enter the name "Cross-Section1" in both input fields.
- ◇ Press the *OK* button.
- ◇ Add the cross section to the network by clicking with the left mouse button on the network.
- ◇ Click the button *Add node* of the menu *Node*: .
- ◇ Enter the name "Cross-Section2" in both input fields.
- ◇ Press the *OK* button.
- ◇ Add the cross section to the network by clicking with the left mouse button on the network.

DELWAQ is the general water quality model of Deltares. DELWAQ can be used stand-alone and in combination with 1D, 2D and 3D-model schematisations. For that reason DELWAQ uses its own schematisation, which can be coupled to any hydraulic model.



Remark:

- ◇ It is essential that a DELWAQ-schematisation is generated!

Perform the following actions

- ◇ Go to the menu *Edit* and subsequently *Delwaq segments*.
- ◇ Click the button *Auto*.
- ◇ Click the menu *File* → *Close*.

The DELWAQ-segments are coloured red in the map.

7.2.1.11 Model data

The input data of the model, i.e. the profiles and the boundary conditions, are to be edited in the menu item 'Model data'.

- ◇ Go to the menu 'Edit' and subsequently to 'Model data'.

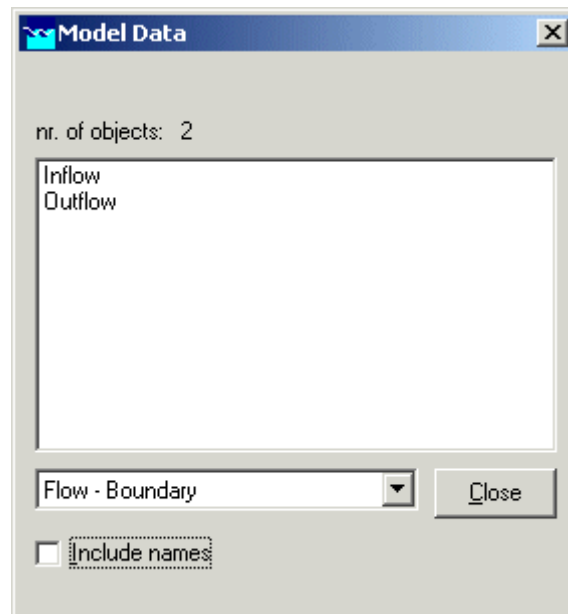


Figure 7.57: The Model Data Window

- ◇ Select the node with the identifier 'Inflow'.
- ◇ Click the *Edit* button that appears in the upper right corner of the 'Model Data' window.

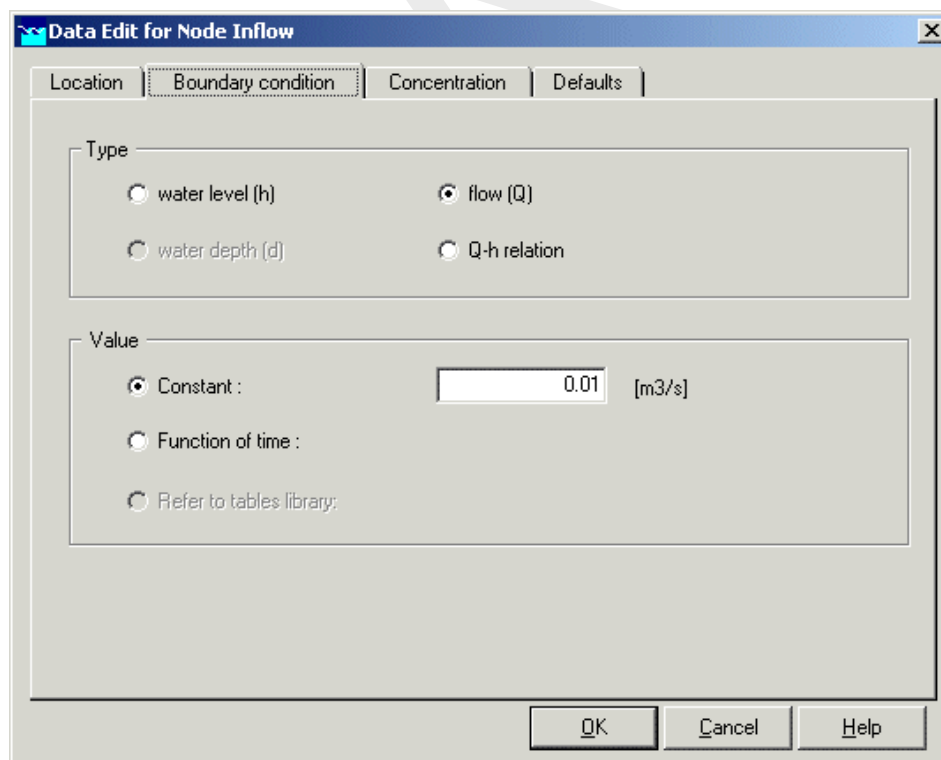


Figure 7.58: The data editor for hydrological data.

- ◇ Go to the tab 'Boundary condition'.
- ◇ Select 'flow (Q)' for this boundary condition.
- ◇ Select constant option for value and enter value "0.01" m^3/s .
- ◇ Go to the tab 'Concentration'.

This 'Data Edit' window offers the functionality to edit both the local concentration definition for the current object and the global concentration definition for the current fraction.

- ◇ Choose the option 'Use local values' at the upper left of the window.
- ◇ **Select 'Show: Local definition for current object'.**
- ◇ Choose the option 'Constant values' for 'Active Substance Concentrations'.
- ◇ Enter the concentrations (you must double click the cells first) as shown in Figure 7.59.

Data Edit for Node Inflow

Location | Boundary condition | **Concentration** | Defaults

Show: Local definition for current object

☒ Use local value(s)

Information
Current fraction: Boundary Flow

Active Substance Concentrations
☒ Constant values
☐ Time dependent

| Substance | Concentration |
|-----------|---------------|
| NH4 | 1 |
| CBOD5 | 0 |
| CBOD5_2 | 1 |
| OXY | 5 |

OK Cancel Help

Figure 7.59: Boundary condition concentrations.

- ◇ Click the *OK* button.
- ◇ Select the boundary node 'Outflow' in the 'Model Data' window.
- ◇ Click the *Edit* button.
- ◇ Go to the tab 'Boundary condition'.
- ◇ Select 'water level (h)' for this boundary condition.
- ◇ Enter a 'constant value' of "9" 'm. above datum'.
- ◇ Go to the tab 'Concentration'.
- ◇ Tick 'Use local values'.
- ◇ **Select 'Show: Local definition for current object'.**
- ◇ Tick 'Constant values'.
- ◇ Enter the concentrations in the table as shown in the figure above.
- ◇ Click the *OK* button.
- ◇ Select the node 'CSO' on the map.
- ◇ Click the right mouse button and select 'Model data' - 'Flow Model'.

At this point the boundary condition of the sewer overflow can be provided. At this moment we enter a discharge of $0 \text{ m}^3/\text{s}$. The reference model simulates the current situation, without sewer overflow.

- ◇ Go to the tab 'Lateral flow'.
- ◇ Enter a constant discharge of "0" m³/s.

In The Netherlands, the waste load from the sewer system to surface water is calculated as the product of the discharge of the overflow and a constant concentration. Realistic concentrations are:

| Substance | Concentration |
|-----------|---------------|
| NH4 | 5.5 mg/l |
| CBOD5 | 60 mg/l |
| CBOD5_2 | 40 mg/l |
| OXY | 7 mg/l |

- ◇ Go to the tab 'Concentration'.
- ◇ Tick 'Use local values'.
- ◇ **Select 'Show: Local definition for current object'.**
- ◇ Tick 'Constant values'.
- ◇ Enter the concentrations of "NH4", "CBOD5", "CBOD5_2" and "OXY" in overflow water in the table.
- ◇ Click the *OK* button.

After the boundary data conditions have been entered, the cross sections are to be defined.

- ◇ Select 'Flow - Cross Section' in the check box in the window 'Model Data'.
- ◇ Select 'Cross-Section1'.
- ◇ Click the 'Edit' button that appears in the upper right corner of the Model Data window.
- ◇ Go to the tab 'Location'.
- ◇ Enter a bed level of "8.5" m above datum.
- ◇ Enter a surface level of "10.5" m above datum.
- ◇ Go to the tab 'Cross section'.
- ◇ Select the trapezium as the general type of cross section to be used.
- ◇ Enter the name "River profile 1" in the input box next to 'Cross section : '.
- ◇ Click *Define dimensions*, for entering the dimensions of the cross section.
- ◇ Enter "2" as the slope.
- ◇ Enter "1.5" meter as the Bottomwidth B.
- ◇ Enter "7" m as the maximum flow width.
- ◇ Click *Save dimensions*. You'll get a warning message which says " *You changed the profile definition. Do you want to add it as a new definition?*".
- ◇ Click the *OK* button.

The result is shown below.

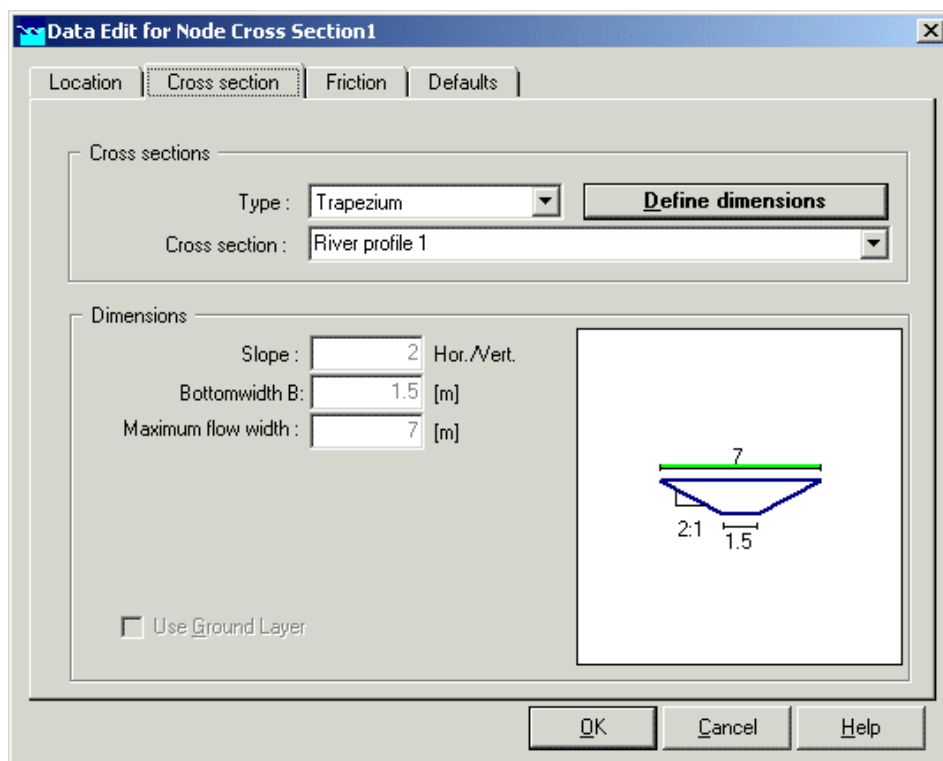


Figure 7.60: Defining the cross section.

- ◇ Go to the tab 'Friction'.

SOBEK offers the functionality to set a global friction value. This value will be used in simulation in case no local friction value has been provided.

- ◇ In the 'Show' list button, select 'Global value(s)'.
- ◇ Select the option 'Chezy' for 'type friction (Bed)'.
- ◇ Enter "40" for constant value.
- ◇ Click the *OK* button.
- ◇ Select the cross section 'Cross-Section2' from the list.
- ◇ Click the *Edit* button.
- ◇ Go to the tab 'Location'.
- ◇ Enter a bed level of "8" m above datum.
- ◇ Enter a surface level of "10" m above datum.
- ◇ Go to the tab 'Cross section'.
- ◇ Select the trapezium as the general type of cross section to be used.
- ◇ Select the 'River profile 1' from the list 'Cross section :'.
- ◇ Click the *OK* button.
- ◇ Click the *Close* button of Model Data.
- ◇ Select 'File' - 'Save' - 'Network' to save the network.
- ◇ Select 'File' - 'Save' - 'Map' to save the map.
- ◇ Select 'File' - 'Exit' to leave NETTER and to return to the 'Schematisation' menu.

7.2.1.12 Simulation of the reference model

- ◇ Click the *OK* button.
- ◇ Double click the task block 'Simulation' in the Case Manager.

Now SOBEK will start the simulation.

7.2.1.13 Presentation of the simulation results

The simulation results can be presented as a table, a graph, or in a map. The presentation in a graph is the best method if you want to judge whether or not appropriate values have been chosen as model parameters.

Results in Charts

- ◇ Double click the task block 'Results in Charts' in the Case Manager.
- ◇ Select 'History Results of Water Quality'.
- ◇ Then click the *View* button.
- ◇ Select the parameter 'OXY' (oxygen).
- ◇ Select a segment halfway the schematisation, for instance segment 10.
- ◇ Click the button *All* above the right table, to have all output time steps shown in the graph.

See also [Figure 7.61](#), where the selected output options are shown.

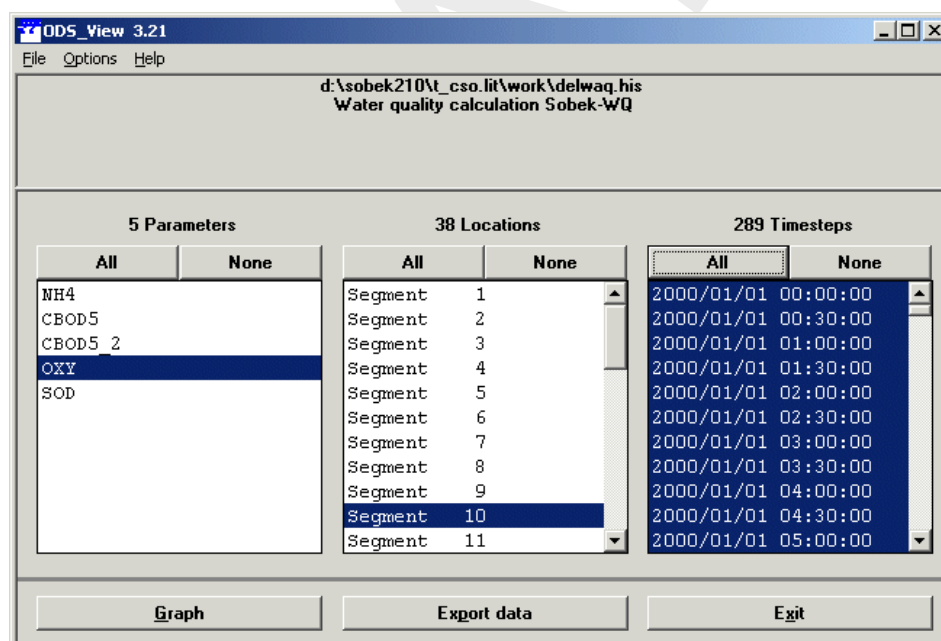


Figure 7.61: Selecting output parameters in 'History Results of Water Quality'.

- ◇ Click the *Graph* button.

As can be seen, the oxygen concentration is increasing slowly in time. The increase is due to re-aeration.

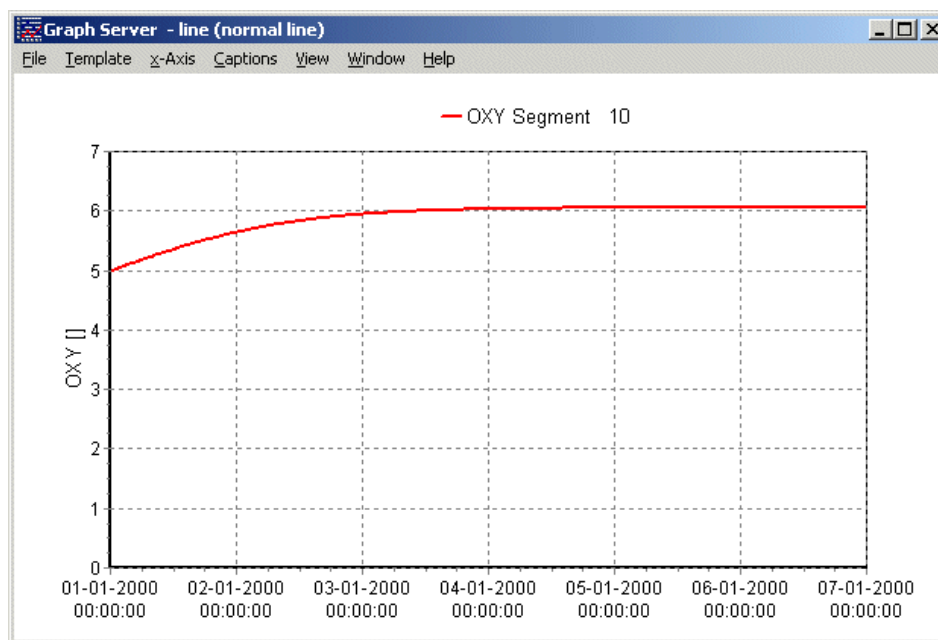


Figure 7.62: The oxygen concentration for the reference situation. (Graph may differ depending on the segment numbering and length of your schematisation)

- ◇ Click 'File' and subsequently 'Exit' to close the figure.
- ◇ Press the *Exit* button.
- ◇ Click the *Exit* button to leave the task block 'Results in Charts'.

Save the model!

Don't forget to save the model! The model can be saved in the Case Manager.

- ◇ Go to the menu 'Case' and subsequently 'Save' to save the case.

7.2.2 Creating cases for several overflow situations

7.2.2.1 The Case manager (I)

In this chapter the reference model for the current situation will be used to create cases for the simulation of the effects of combined sewer overflows with repeat times of 1, 2, 5 and 10 year. This can be done in the Case Manager.

Note that the case 'Reference model' is saved under new names. The copies of the reference case are used to simulate the effects of sewer overflows with different repeat times.

Please be aware that the Case Manager makes a copy of the model! There is no direct link with the reference model anymore! A change in the network schematisation (for instance river discharge) has to be made in all cases, in order to avoid differences between the cases.

- ◇ Go to the menu 'Case' and then 'Open as new'.
- ◇ Select the case 'Reference model'.
- ◇ Enter the name "T1".
- ◇ Press the *OK* button.

7.2.2.2 Model data

A sewer overflow is in general a peak discharge that lasts for some hours. The sewer overflow will be modelled as a boundary condition for the node with lateral discharge. In order to give the model some start-up time, the overflowing happens at the third day.

- ◇ Double click the task block 'Schematisation'.
- ◇ Click *Edit model* in the 'Schematisation' menu.
- ◇ Select the node 'CSO' on the map.
- ◇ Click the right mouse button.
- ◇ Select 'Model data' - 'Flow Model'.
- ◇ Go to the tab 'Lateral Flow'.
- ◇ Choose for a 'Function of time'.
- ◇ Click the *Table...* button.
- ◇ Press the *Add Row* button.
- ◇ Enter "3".
- ◇ Press the *OK* button.
- ◇ Enter the time series as shown below.

| | Date [dd/mm/yyyy] | Time [hh:mm:ss] | Discharge [m3/s] |
|---|----------------------|--------------------|---------------------|
| 1 | 01/01/2000 | 00:00:00 | 0 |
| 2 | 03/01/2000 | 00:00:00 | 0.1 |
| 3 | 03/01/2000 | 03:00:00 | 0 |
| 4 | 31/01/2000 | 00:00:00 | 0 |

Options:

☒ Block function ☐ Linear function

☐ Use periodicity of

Figure 7.63: The time series of the sewer overflow for the case 'T1'.

- ◇ Tick the option 'Block function'.
- ◇ Click the *OK* button to close the 'Edit Table'.
- ◇ Press the *OK* button to close the 'Data Edit for Node' window.
- ◇ Go to the menu 'File' and then 'Save' and finally 'Network' to save the changes.
- ◇ Go to the menu 'File' and then Exit to leave NETTER.
- ◇ Click the *OK* button to leave the 'Schematisation' and to return to the Case Manager.

The discharge of the sewer overflow with a repeat time of 1 year has been entered now.

7.2.2.3 The Case Manager (II)

The changes in the case 'T1' must be saved by the case manager.

- ◇ Go to 'Case' and then 'Save' to save the case.
- ◇ Go to 'Case' and then 'Close' to close the case.

Now that the case has been saved, you should make copies of the reference case again by using the Open as New option in the Task Manager, selecting the T1 case and choosing a new case name for 3 new cases as listed below.

| name of the case | repeat time | CSO discharge | duration of the event |
|------------------|----------------|-----------------------------|-----------------------|
| reference model | — | — | — |
| T1 | (T = 1 year) | $0.10 \text{ m}^3/\text{s}$ | 3 hours |
| T2 | (T = 2 years) | $0.20 \text{ m}^3/\text{s}$ | 3 hours |
| T5 | (T = 5 years) | $0.50 \text{ m}^3/\text{s}$ | 3 hours |
| T10 | (T = 10 years) | $0.75 \text{ m}^3/\text{s}$ | 3 hours |

- ◇ Set up the schematisation of the three remaining cases T2, T5 and T10 in the same way you modelled the case T1. Each case will have a different discharge value for the 'CSO' node representing a different repeat time.



Remarks:

- ◇ The above repeat time is listed for the purpose of clarifying the tutorial data. The repeat time is not actually a value that the user can enter during this tutorial.
- ◇ Do not forget to save each case before you make a copy or close them!

7.2.3 Simulations in batch mode

Since there are different cases to be calculated, it would be easy if those simulations were made in series, without the need for modeller intervention. For this reason, SOBEK offers the option of simulating in batch mode.

7.2.3.1 Simulations

First we have to specify the cases that must be simulated in a batch.

- ◇ Close the case, if one is loaded at the moment, via the menu *Case* and subsequently *Close*.
- ◇ Go to the menu *Case* and then to *Define Batch*.

In the window shown below the batch can be specified

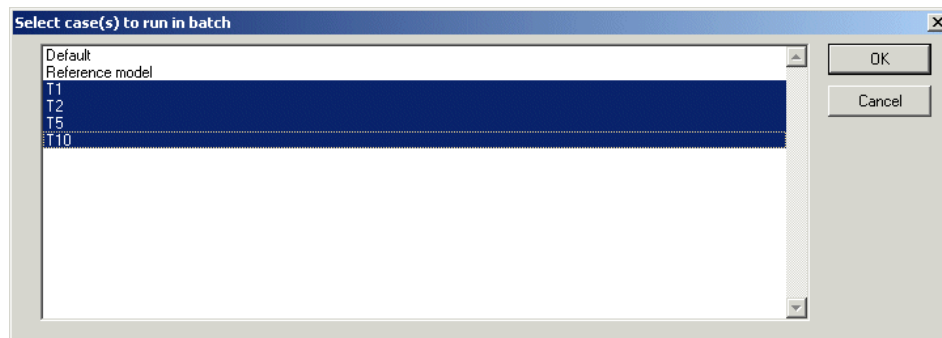


Figure 7.64: Specifying the batch simulation.

- ◇ Select the cases 'T1', 'T2', 'T5' and 'T10', by clicking while the `Ctrl` key is kept pressed.
- ◇ Click the *OK* button.
- ◇ Click the grey task block 'Simulation'. The task block becomes surrounded by an orange margin.
- ◇ Go to *Case* and *Run Batch*.

The simulations are made and saved one by one now.

7.2.3.2 Special settings

It can happen that the simulations in batch mode are interrupted by the message shown below:

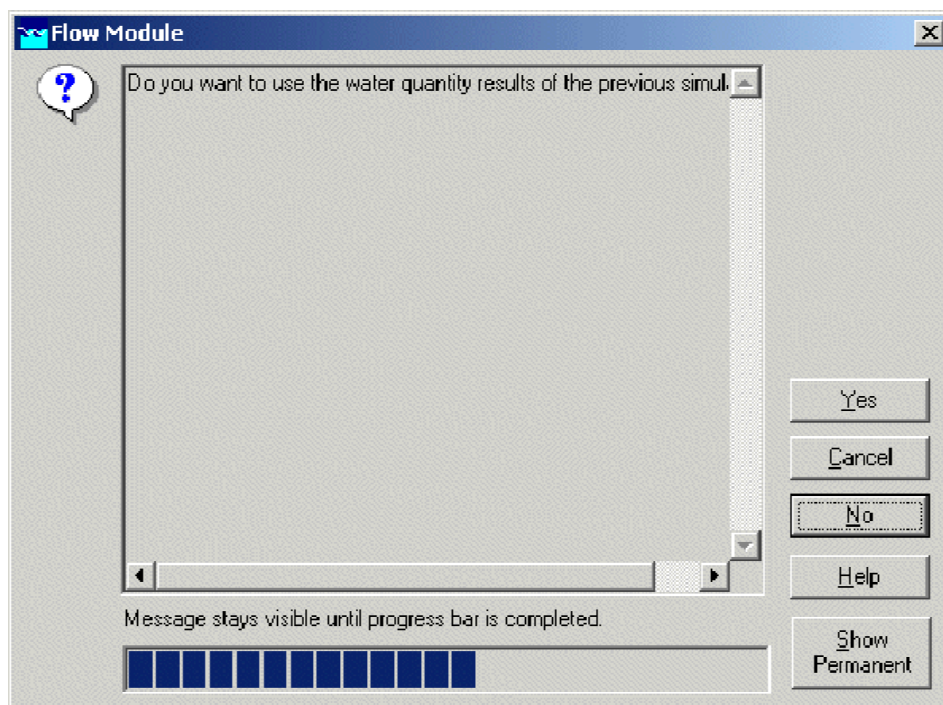


Figure 7.65: Using the previous simulation results.

A window with such a question would halt the calculation, until an answer is given. For this reason a timer has been incorporated: after two minutes the window disappears and the simulation continues. Default the answer is 'No'. After thirty seconds of waiting a new flow simulation is started. Of course you can also click 'No' yourself. It's important that the flow simulation is renewed, because the available flow results stem from the reference model that has been copied!

By switching on the option 'use previous flow results in batch mode' in 'Settings', 'water quality', on the tab 'Simulation options', the default answer becomes 'Yes'. This can save calculation time. However, to avoid confusion, it's recommended that this option is not used for the example in this tutorial.

- ◇ Press the *No* button four times.

7.2.4 Presentation and analysis of the results

With the Case Analysis Tool the results of several cases can be compared with each other and shown in one graph or map. This is of great help while analysing several scenarios or situations. For instance when you want to compare the oxygen concentration in the surface water after a number of sewer overflow events. Furthermore the Case Analysis Tool (CAT) offers many (statistical) functions, like the derivation of minima and maxima, averages, deviation from the required water quality etc.

7.2.4.1 Making a graph in the Case Analysis Tool (CAT)

With the sewer overflows in these cases one might expect that more oxygen will be depleted at events with a higher repeat time. This can be demonstrated with a figure at one location in which the oxygen concentration is shown for several repeat times. Such a graph can be made in the Case Analysis Tool.

- ◇ Leave the Case Manager via 'Case' and then 'Exit'.
- ◇ Select 'Projects' - 'Case Analysis Tool'.
- ◇ Select the project 'T_CSO'.
- ◇ Click the OK button.
- ◇ Go to the tab 'Cases'.
- ◇ Select the case T1 in the left panel. Select the function 'WQ: history results' in the right half of the window.
- ◇ Do the same for the cases 'T2', 'T5', en 'T10': select the name of case an click on the function 'WQ history results' in the right half of the window.

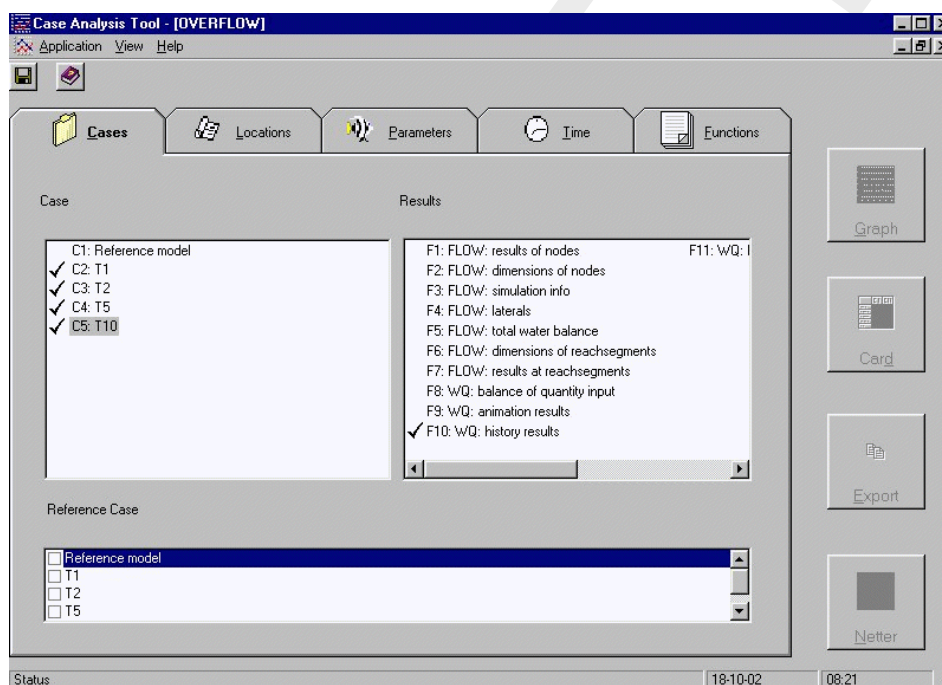


Figure 7.66: The Case Analysis Tool.

- ◇ Go to the tab 'Locations'. If the tab names are not visible, increase the width of the window.
- ◇ Select a segment (for example, segment 33) in the left column and click the button '>'.
- ◇ Go to the tab 'Parameters'.
- ◇ Select 'OXY' and click '>'.
- ◇ Note: Neither on the tab 'Time', nor on the tab 'Functions' changes have to be made.
- ◇ Click the button 'Graph', at the right side of the window.

Remark:

- ◇ The amount of delwaq segments in this network is determined by the distance between the two boundary nodes we placed earlier in this tutorial. Depending on where exactly the boundary nodes were placed, both the amount of delwaq segments in this network may vary, as may the results for any specific delwaq segment.



A graph with simulated oxygen concentration after the four events appears.

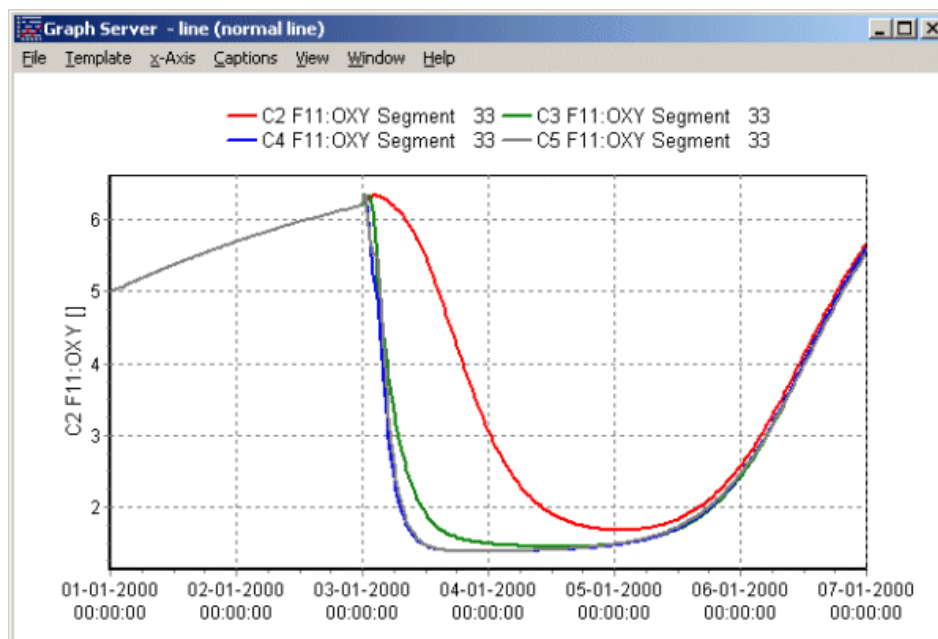


Figure 7.67: The simulation results of oxygen after four events with repeat times T_1 , T_2 , T_5 and T_{10} .


- ◇ Close the graph server window via 'File' and 'Exit'.
- ◇ Leave the Case Analysis Tool via the menu 'Application' and 'Exit'.
- ◇ Press the No button.

7.2.4.2 Results in maps

The previous paragraph showed that the effects of the sewer overflow are most pronounced after overflow events with repeat times of 5 and 10 years. In this paragraph the simulation results of the case T_{10} will be analysed further.

- ◇ Click in the main SOBEK menu on 'Open Project'.
- ◇ Choose the project 'T_CSO'.
- ◇ Press the OK button.
- ◇ Select 'Case' - 'Open'
- ◇ Select the case 'T10'.
- ◇ Press the OK button.
- ◇ Double-click the task 'Results in Maps' and NETTER will start.
- ◇ Select 'Map Results of Water Quality' in the Active Legend.

To get a quick overview of the results data, you can make the nodes change colour and size, according to their data value.

- ◇ Choose 'Options' - 'Network Data...' in the menu bar.
- ◇ Click the 'All Data' tab.
- ◇ Activate the 'Width' checkbox for 'Show branch data'.
- ◇ Click the OK button.
- ◇ Select 'OXY' in the View Data list.
- ◇ Change the 'Play mode' in the menu 'play mode' into 'Play Continuous'
- ◇ Click the button  in 'View Data' and the oxygen concentration in the canal is shown as

a movie.

A map with the minimum oxygen concentration that is simulated is very illustrative, because it shows the influence sphere of the sewer overflow.

- ◇ Go to the menu 'Options' - 'Data Statistics' and select 'minimum'.

For presentation purposes it might be useful to customise the scale:

- ◇ Go to the menu 'Options' - 'Data value options'
- ◇ Tick the option 'User'.
- ◇ Click the button 'Scale'.

In this window you can customise the scale: the number of classes, boundaries of classes and colours.

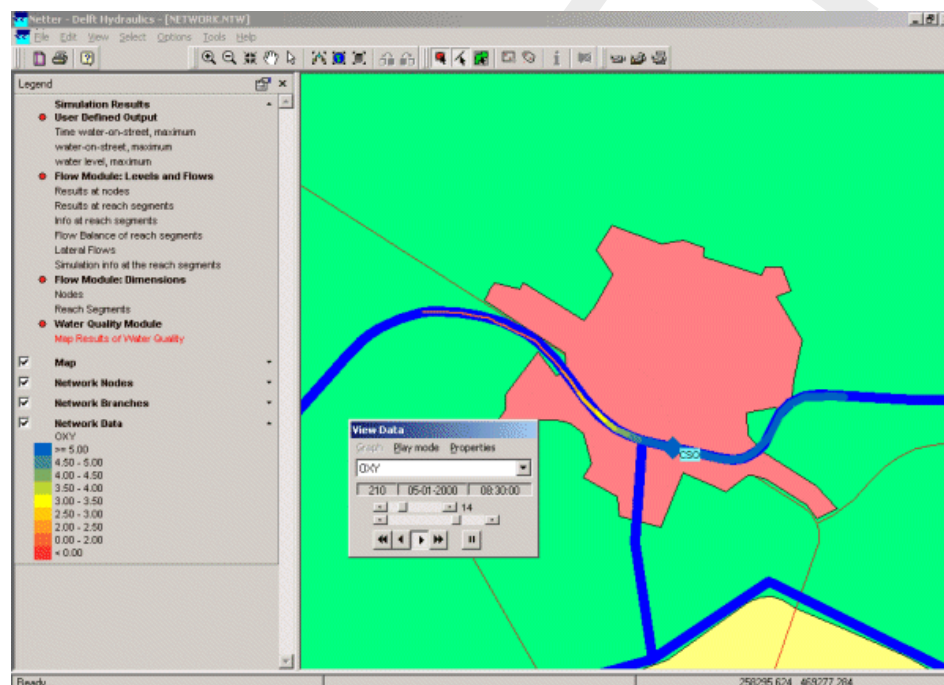


Figure 7.68: The simulation results of oxygen after an event with a repeat time of 10 years. The minimum oxygen concentration is shown.

- ◇ Click the OK button.
- ◇ Click the OK button.
- ◇ Select 'File' - 'Exit' to leave NETTER.
- ◇ Select 'Case' - 'Close'.
- ◇ Press the Yes button.

7.2.5 Fraction calculations

The option 'Fraction calculations' is a useful tool for the analysis of the transport and dispersion of water through the water system. The water flowing from each source is labelled, for instance as River water, Overflow water and Initial water. In this way the origin of the water at a certain point in the water system can be traced back to the source.

7.2.5.1 Settings

- ◇ Select 'Case' - 'Open as new'.
- ◇ Select the case 'T1'.
- ◇ Enter the name "Fraction T1".
- ◇ Press the *OK* button.
- ◇ Double click the task block 'Settings'.
- ◇ Click the button 'Edit' next to '1DWAQ'.
- ◇ Go to the tab 'WQ Processes'.
- ◇ Select 'calculate fractions'.
- ◇ Click the *OK* button to leave the 1DWAQ Settings.
- ◇ Click the *OK* button to return to the Case Manager.

7.2.5.2 User defined objects

The water fractions enter the water system via so-called user defined objects. The user defined objects are copies of existing object types like 'Flow-Boundary' and 'Flow-Lateral Flow', but have a unique water fraction. In this model three water fractions are discerned: River water, Sewer water and Initial water. The boundary nodes where these fractions enter the water system will be defined by the modeller.

- ◇ Double click the task block 'Schematisation'.
- ◇ Click the *Edit User Defined Objects* button.

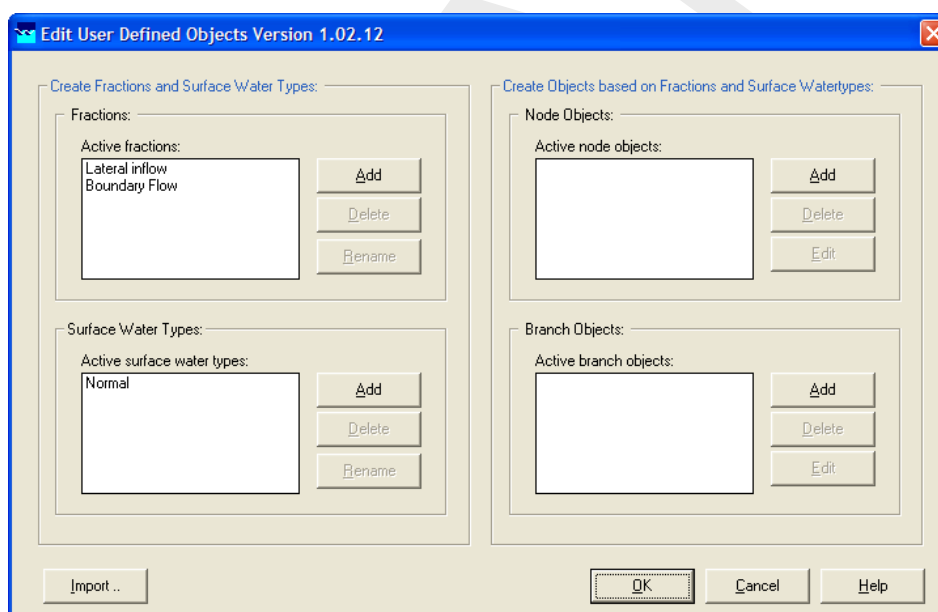


Figure 7.69: In this window the 'User Defined Objects' are created.

The window in [Figure 7.69](#) appears. This window consists of four fields. First the water fractions will be defined. Then these fractions are coupled to objects. These new, user defined objects can be applied in the model schematisation. In this specific example two objects will be added to the list with object types: an object for the upstream boundary and an object for the sewer overflow.

- ◇ Click the *Add* button next to the input block 'Active fractions' (upper left input block).
- ◇ Enter the name of the fraction: "River water".
- ◇ Click *OK* button.
- ◇ Click the 'Add' button once again, to add a second fraction.

- ◇ Enter the name of the fraction: "Sewer water".
- ◇ Click *OK* button.
- ◇ Click *Add* next to the input block 'Active node objects' (upper right block).

Figure 7.70: Defining a new Node object.

The window in [Figure 7.70](#) appears. In this window the new objects are given a name. The objects are linked with a water fraction. Furthermore one has to specify the type of object that the new object is derived from.

- ◇ Enter the 'Object name': "River node".
- ◇ Select the type of node where the new node is derived from: 'Flow - Boundary'.
- ◇ The 'Selected fraction' is the fraction 'River water'.
- ◇ Click the *OK* button.
- ◇ Click *Add* next to the input block 'Active node objects' once again.
- ◇ Enter the 'Object name': "Overflow node".
- ◇ Select the type of node where the new object is derived from: 'Flow - Lateral Flow'.
- ◇ The 'Selected fraction' is the fraction 'Sewer water'.
- ◇ Click the *OK* button.
- ◇ Click the *OK* button to return to the 'Schematisation' menu.
- ◇ Click the *Edit model* button and NETTER will be started.

Remark:

- ◇ After modifying User-defined objects, the user must always open the network editor and save the network again. If this step is not performed, the modified user-defined objects will not be fully updated.



7.2.5.3 Preparation of the network

The new objects have to be included in the network. In this way two new sources of water are introduced in the fraction calculations: River water and Sewer water.

- ◇ Zoom in on the CSO node.
- ◇ Click the button 'Edit Network'.

Your Flow Mode node menu will now look similar to [Figure 7.71](#).

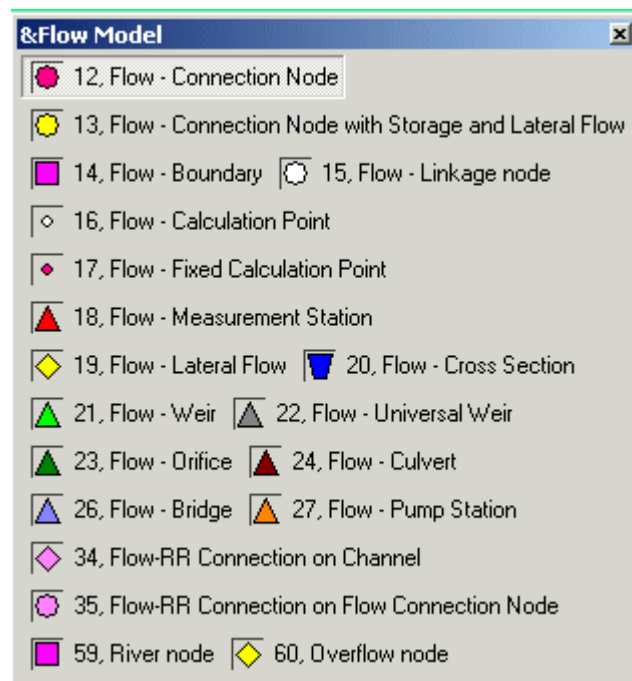







Figure 7.71: The available objects. At the bottom are two new user defined objects: 'River node' and 'Overflow node'.

From now on two new user defined objects are available: 'River node' and 'Overflow node'. In the network two existing objects will be replaced by these two new nodes.

In order to see the objects on the map please:

- ◇ Click the  button in the Active Legend or select the menu item 'Options' - 'Network Data...'.
 - ◇ Select the tab 'Node'.
 - ◇ Select the radio button 'Netter Type'.
 - ◇ Press the *OK* button.
- ◇ Click the object type 'Overflow node' in the menu 'Node': .
- ◇ Click the button 'Node type' of the menu 'Node': .
- ◇ Click the CSO node, that represents the Sewer Overflow. This node is replaced by a node of the object type 'Overflow node'.
- ◇ Zoom in on the 'Inflow' node.
- ◇ Click the object type 'River node' in the menu 'Node': .
- ◇ Click the button 'Node type' of the menu 'Node': .

- ◇ Click the 'Inflow' node that represents the upstream river boundary. This object is replaced by an object of the type 'River node'.

Now, we will check if the hydrological data of the replaced nodes is still correct. Please note that the boundary conditions for water quality (i.e. the concentrations at the boundaries) are no longer visible. This is because fraction calculations don't use them.

- ◇ Go to the menu 'Edit' - 'Model Data'.
- ◇ Select the 'Overflow node' option.
- ◇ Select the node 'CSO'.
- ◇ Click the 'Edit' button that appears in the upper right corner of the window.
- ◇ Have a look at the boundary conditions with regard to the water quantity.
- ◇ Click the *OK* button.
- ◇ Select the 'River node' option.
- ◇ Select the node 'Inflow'.
- ◇ Click the 'Edit' button that appears in the upper right corner of the window.

Have a look at the boundary conditions with regard to the water quantity. As you can see, the model data of the original boundary condition has been copied into the user defined object, "River node".

When you are finished looking at the data:

- ◇ Click the *OK* button.
- ◇ Go to the menu 'File' - 'Save' - 'Network'.
- ◇ Go to the menu 'File' - 'Exit' to leave NETTER.
- ◇ Click the *OK* button in the Schematisation menu' to return to the Case Manager.

7.2.5.4 Simulation and presentation of the results

- ◇ Double click the task block 'Simulation'.
- ◇ Press the *No* button.
- ◇ Click the task block 'Results in Charts' when the calculation is finished.
- ◇ Choose for 'History Results of Water quality'.
- ◇ Press the *View* button.

The window shown below appears. In total four fractions, the volume and a check are shown. Two of them have been added in the previous chapter.

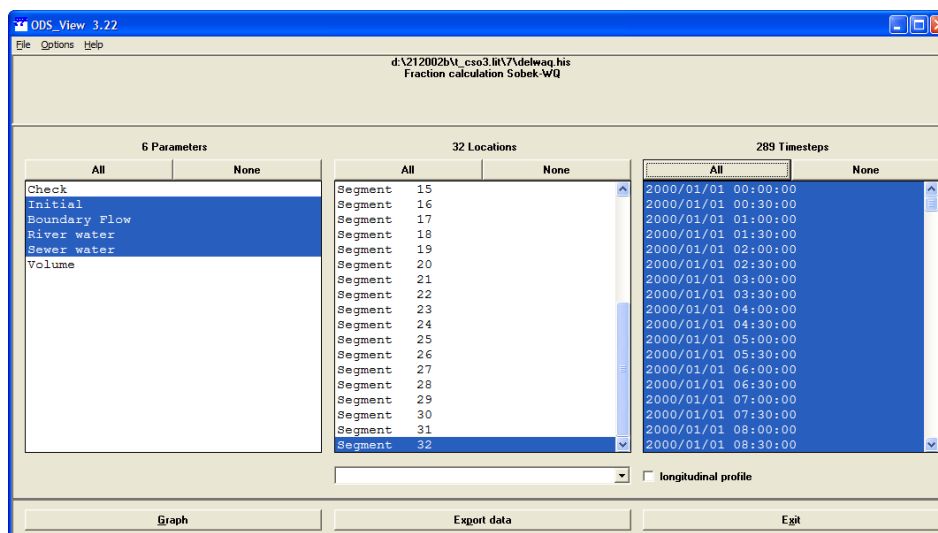


Figure 7.72: Preparing a graph.

- ◇ Select the fractions 'Initial', 'Boundary Flow', 'Sewer water' and 'River water', by clicking them while the **Ctrl** key is kept pressed.
- ◇ Select a segment, for example segment 32.
- ◇ Click *All* above the table with the output time steps to select the entire simulation period.
- ◇ Click the *Graph* button.
- ◇ Go to the menu 'Template' and choose for 'area (stacked area)'.

The results of the fraction calculation are shown in [Figure 7.73](#). In the example output, the influence of the sewer overflow on segment 32 is clearly visible down from day 3. The initial water is driven out of the initial water by River water and by Sewer water.

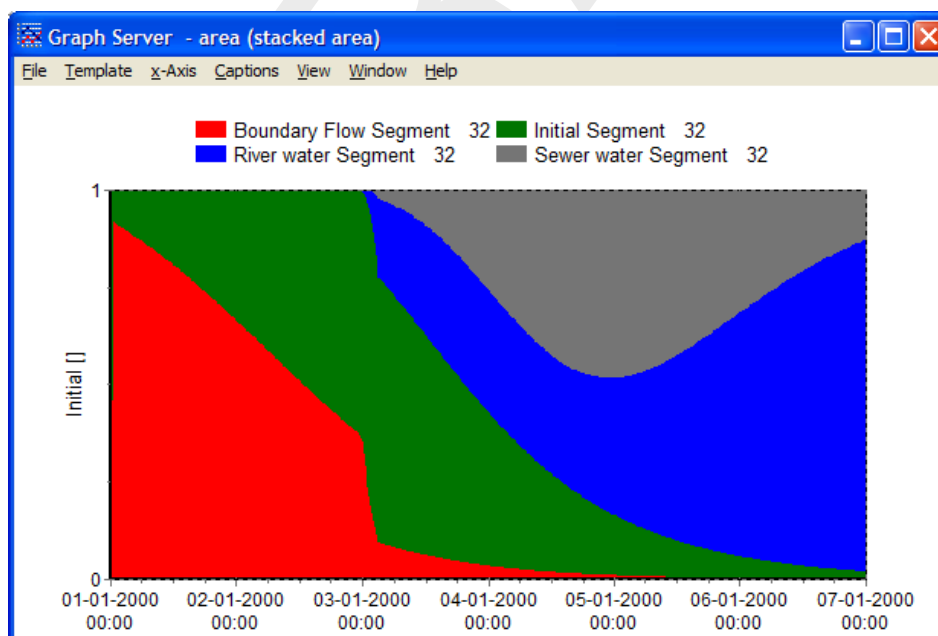


Figure 7.73: The results of the fraction calculations.

- ◇ Go to the menu 'File' - 'Exit' to close the figure.
- ◇ Click the *Exit* button.
- ◇ Click the *Exit* button to return to the Case Manager.

- ◇ Go to 'Case' and then 'Save' to save the case.
- ◇ Go to 'Case' and then 'Close' to close the case.
- ◇ Go to 'Case' and then 'Exit' to return to the main menu of SOBEK.

7.2.5.5 Epilogue

In this example the fraction calculations were set up after the network was created and several calculations were made. This approach was chosen for educational reasons. You may save time if you define the 'user defined objects' before you start to make a schematisation.

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8 Conceptual description

8.1 Introduction

D-WAQ 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-WAQ 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-WAQ. 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-WAQ and the underlying principles of how to describe transport and water quality processes.

8.2 Mass balances

D-WAQ 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-WAQ solves Eq.(8.1) for each computational cell and for each state variable. Eq.(8.1) is a simplified representation of the advection-diffusion-reaction equation which will be discussed in [section 8.4](#).

$$M_i^{t+\Delta t} = M_i^t + \Delta t \times \left(\frac{\Delta M}{\Delta t} \right)_{Tr} + \Delta t \times \left(\frac{\Delta M}{\Delta t} \right)_P + \Delta t \times \left(\frac{\Delta M}{\Delta t} \right)_S \quad (8.1)$$

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-WAQ 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-WAQ has to solve Eq.(8.1).

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 hydrodynamic model (Delft3D-FLOW UM, 2013). Dispersion in the vertical direction which is important if the water column is stratified, is derived from Delft3D-FLOW as well. Dispersion in the horizontal direction is user input (refer to section 5.3.3). 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 Delft3D-FLOW).

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-WAQ refer to chapter 9 and the D-WAQ Technical Reference Manual (D-WAQ TRM, 2013).

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 Delft3D-FLOW hydrodynamic model.

8.3 Spatial schematisation

To model the transport of substances, a water system is divided in small boxes (Figure 8.1). The complete ensemble of all the small boxes is called the 'grid' or 'schematisation'. In D-WAQ 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.

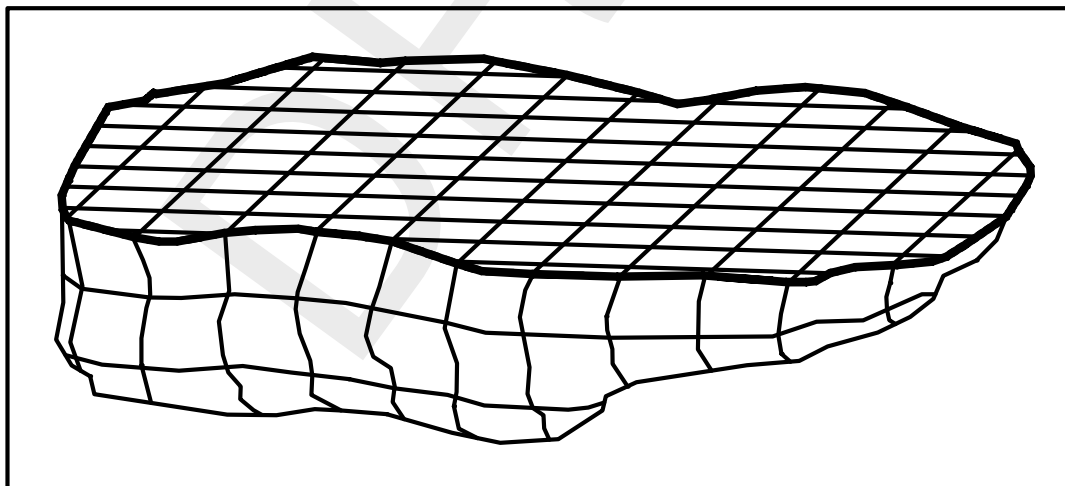


Figure 8.1: Division of a lake into small boxes with a finite volume; a structured three dimensional grid is used

In D-WAQ 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-WAQ 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-WAQ 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-WAQ is shown in Figure 8.2.

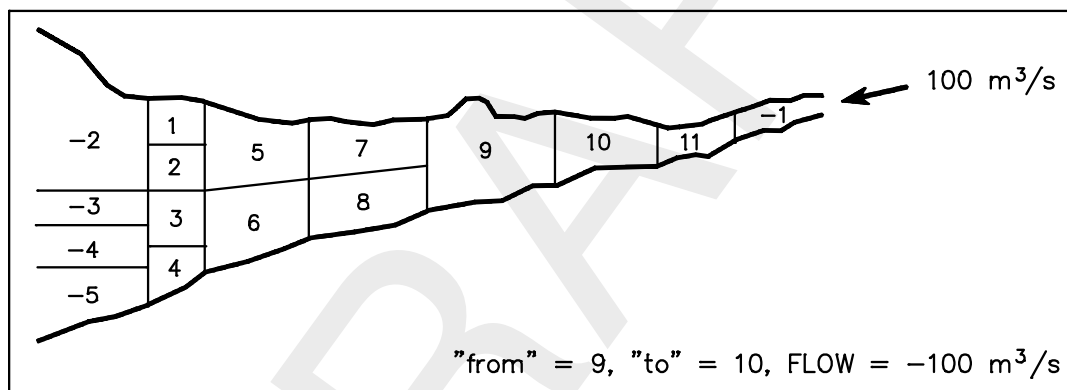


Figure 8.2: Schematisation of an estuary with 11 computational cells and 5 boundary cells indicated with a negative number. The exchange table indicates how the computational cells are connected to each other and what the flow between the computational cells is. The "From-1" and "To+1" columns refer 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.

8.4 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-WAQ makes this mass balance for you, for so-called *segments* (i.e. small water volumes):

$$\frac{\partial M}{\partial t} = \text{advection} + \text{dispersion} + \text{source} \quad (8.2)$$

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

8.4.1 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.

8.4.2 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.

8.4.3 Transport from sources

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

$$T_{src} = Q_{src} \times C_{src} \quad Q_{src} > 0 \quad (8.3)$$

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

$$T_{src} = Q_{src} \times C_i \quad Q_{src} < 0 \quad (8.4)$$

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.

8.4.4 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:

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

with:

| | |
|---|--|
| M_i^t | mass in volume i at time t [g] |
| Δt | time step [s] |
| $\frac{\partial C}{\partial x} \Big _{x_0}$ | 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-WAQ uses the following *equivalent* equation:

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

with:

| | |
|---|--|
| M_i^t | mass in volume i at time t [g] |
| Δt | time step [s] |
| $\frac{\partial C}{\partial x} \Big _{x_0}$ | 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.

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

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

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

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 .

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

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:

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} - D_x \frac{\partial^2 C}{\partial x^2} + v_y \frac{\partial C}{\partial y} - D_y \frac{\partial^2 C}{\partial y^2} + v_z \frac{\partial C}{\partial z} - D_z \frac{\partial^2 C}{\partial z^2} = 0 \quad (8.5)$$

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} - D_x \frac{\partial^2 C}{\partial x^2} + v_y \frac{\partial C}{\partial y} - D_y \frac{\partial^2 C}{\partial y^2} + v_z \frac{\partial C}{\partial z} - D_z \frac{\partial^2 C}{\partial z^2} = S + f_R(C, t) \quad (8.6)$$

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 (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.

8.5 Boundary conditions

8.5.1 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.

8.5.2 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 Delft3D-FLOW, 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-WAQ 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 8.2](#) 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

8.5.3 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-WAQ enables you to use a cosine shaped function from the last outflow concentration to the specified boundary condition, according to [Figure 8.3](#). 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.

In mathematical form it is given by:

$$C(t_0 + t) = C(t_0) \left(0.5 + 0.5 \cos \left(\frac{\pi t}{2T} \right) \right) + C_B(t) \left(0.5 - 0.5 \cos \left(\frac{\pi t}{2T} \right) \right) \quad (8.7)$$

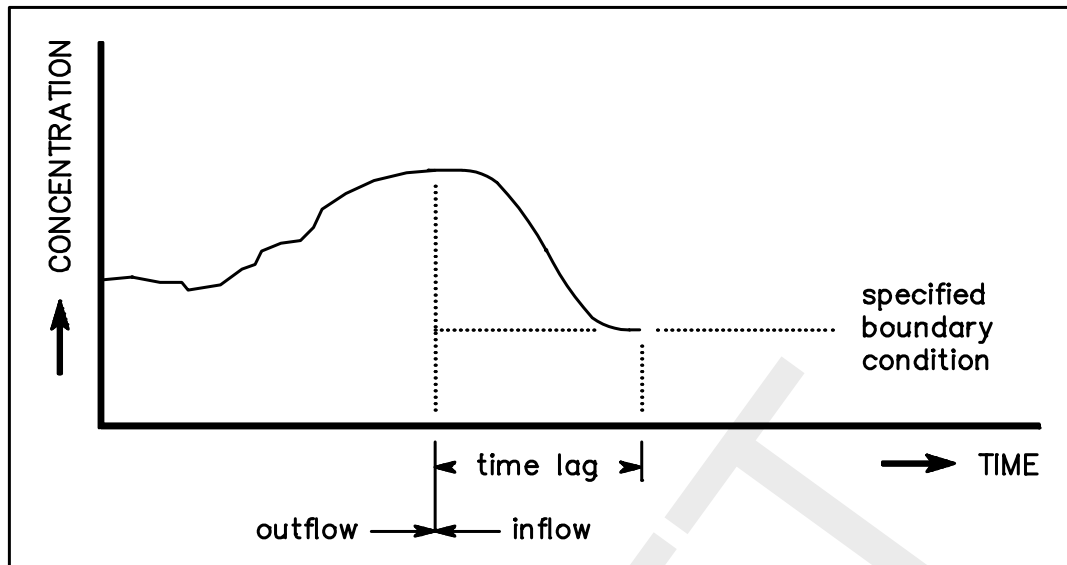


Figure 8.3: Thatcher-Harleman boundary time lag

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

9 Principles of water quality modelling

9.1 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-WAQ 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-WAQ. 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-WAQ model.

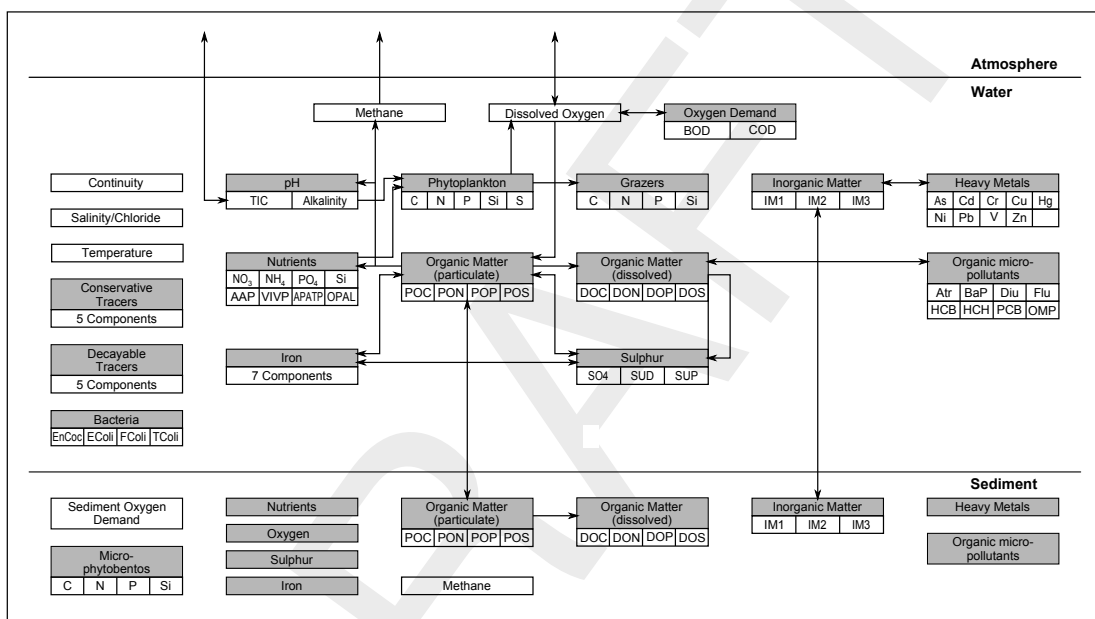


Figure 9.1: General overview of substances included in D-WAQ. Substances are organised in functional groups indicated by a grey header, except for some substances that form a group of their own. Major links between substances are indicated by arrows; note that many links are omitted.

In D-WAQ the constituents of a water system are divided in functional groups (Figure 9.1). 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.

9.2 Salinity, chloride, tracers and continuity

Salinity, chloride and conservative tracers are special substances in D-WAQ 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-WAQ 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/m^3 to all water sources (initial condition, boundary condition and discharges) the Continuity concentration should remain 1 g/m^3 during the whole simulation, as there are no processes that dilute or concentrate it and all water has a concentration of 1 g/m^3 . If the concentration during the simulation significantly deviates from 1 g/m^3 , 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/m^3 , 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-WAQ 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.

9.3 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 \(9.1\)](#) that is applied in many of the processes included in D-WAQ:

$$k = k^{20} \times k_T^{(T-20)} \quad (9.1)$$

with:

| | |
|----------|--|
| k | rate constant at temperature T [d^{-1}] |
| k^{20} | rate constant at reference temperature $20 \text{ }^\circ\text{C}$ [d^{-1}] |
| k_T | temperature coefficient [-] |
| T | ambient water temperature [$^\circ\text{C}$] |

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

D-WAQ 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, Delft3D-FLOW (D-Flow FM UM, 2015; Delft3D-FLOW UM, 2013).

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-WAQ as a segment (forcing) function.



9.4 Coliform bacteria

9.4.1 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.

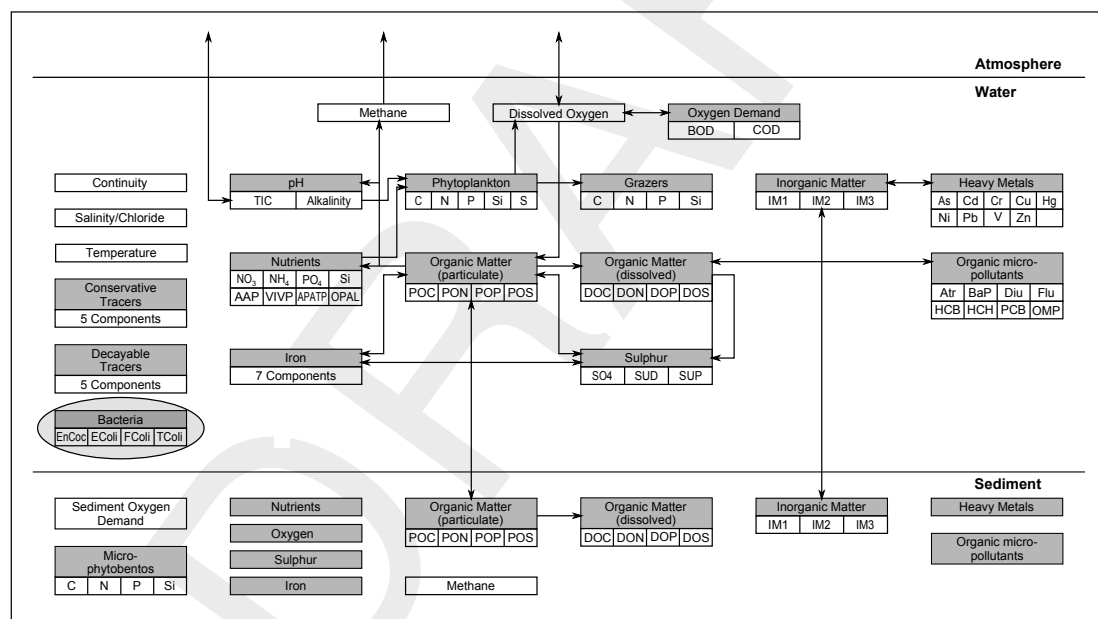


Figure 9.2: Overview of substances. Coliform bacteria

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, ultraviolet radiation in particular.

9.4.2 Modelling framework

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

| Name of D-WAQ 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:

C = concentration of coliform bacteria cells [MPN/m³]
 t = time [day]

9.4.3 Process equation

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

Cx concentration of coliform bacteria species [MPN m⁻³]
 I daily solar UV-radiation at the water surface [W m⁻²]
 kcl chloride related mortality constant [m³ g⁻¹ d⁻¹]
 kmb basic mortality rate [d⁻¹]
 $kmcl$ 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.

9.5 Dissolved oxygen and BOD

9.5.1 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.

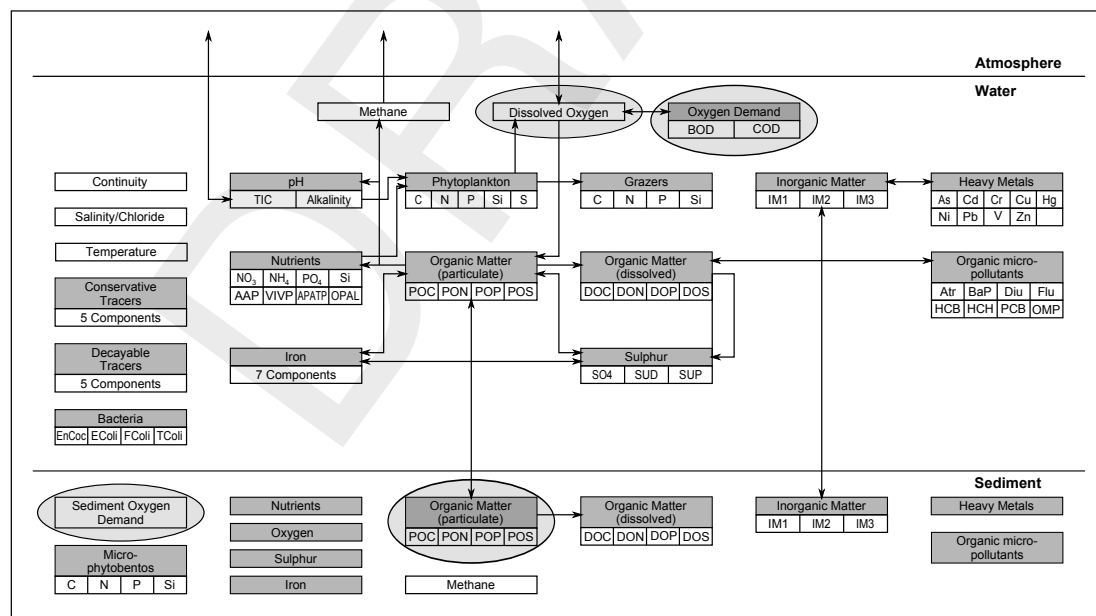


Figure 9.3: Overview of substances. Dissolved oxygen and BOD

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-WAQ.

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 9.1: 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 |

9.5.2 Modelling framework

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

| Name of D-WAQ 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 9.3, 9.4 and 9.5 respectively. The mass balance for CBOD5 is the same as the mass balances for CBODu, NBOD5, NBODu and COD.

$$\frac{\Delta O_2}{\Delta t} = \text{loads} + \text{transport} + \text{reaeration} + \text{net primary production} - \text{mineralization} - \text{nitrification} + \text{denitrification} \quad (9.3)$$

$$\frac{\Delta CBOD5}{\Delta t} = \text{loads} + \text{transport} - \text{settling} - \text{mineralization} \quad (9.4)$$

$$\frac{\Delta SOD}{\Delta t} = \text{loads} + \text{settling} - \text{mineralization} \quad (9.5)$$

In D-WAQ 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 [g O₂/m³]

- 2 Detritus organic carbon originating from natural sources such as dead phytoplankton [g C/m³]
- 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 9.7](#). D-WAQ 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-WAQ 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 gO₂/gC. |
| Nitrification ³ | OXY (NH ₄) (NO ₃) | $NH_4^+ + 2O_2 \rightarrow NO_3^- + 2H^+ + H_2O$ <ul style="list-style-type: none"> ◇ The oxygen consumption is proportional to a nitrification rate and a function of the DO and ammonium concentration. |
| continued on next page | | |

¹ For a description of the settling process refer to [section 9.6](#)

² For a detailed description of sediment processes refer to [section 9.11](#)

³ For process equations refer to [section 9.7](#)

continued from previous page

| Process | Substances | Comments |
|------------------------------------|--|---|
| Denitrification ⁷ | OXY (NO ₃) | $NO_3^- + H^+ \rightarrow 0.5N_2 + 1.25O_2 + 0.5H_2O$ <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. ◇ All fractions in the water column are combined into SOD after settling to the sediment. |

Remarks:

- ◇ All reaction rates are temperature dependent ([section 9.3](#)).
- ◇ 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-WAQ 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.

9.5.3 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 [$\text{gO}_2 \text{ m}^{-3}$] |
| C_{oxs} | saturation dissolved oxygen concentration [$\text{gO}_2 \text{ m}^{-3}$] |
| H | depth of the water column [m] |
| k_{lrear} | reaeration transfer coefficient in water [d^{-1}] |
| R_{rear} | reaeration rate [$\text{gO}_2 \text{ m}^{-3} \text{ d}^{-1}$] |
| SAL | salinity [kg m^{-3}] |
| T | water temperature [$^{\circ}\text{C}$] |
| 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).

Diurnal variation of production

The phytoplankton models implemented in D-WAQ 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 9.4](#). 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:

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

with:

| | |
|----------------|--|
| DL | day length [hr] |
| R_{gp_a} | 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] |

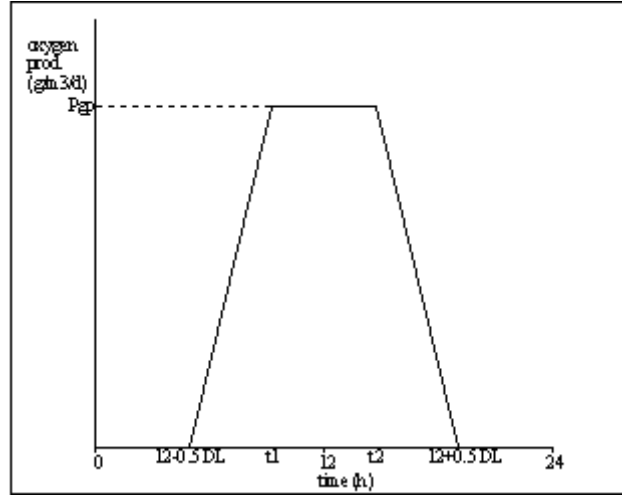


Figure 9.4: The distribution of gross primary production over a day

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:

$$R_{min} = f_{age} \times k_{min} \times Cx \quad (9.6)$$

$$f_{age} = f_{age_{min}} + (f_{age_{max}} - f_{age_{min}}) \times e^{f(AI)} \quad (9.7)$$

$$AI = \frac{COD}{BOD5} \quad (9.8)$$

with:

| | |
|-----------|---|
| AI | index for the age of organic matter [-] |
| Cx | concentration of a BOD/COD-component [$gO_2 m^{-3}$] |
| $BOD5$ | concentration of total CBOD5 [$gO_2 m^{-3}$] |
| COD | concentration of total COD [$gO_2 m^{-3}$] |
| f_{age} | attenuation function for age [-] |
| k_{min} | first-order kinetic constant [d^{-1}] |
| R_{min} | mineralization rate of a BOD/COD-component [$gO_2 m^{-3} d^{-1}$] |

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:

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

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 [$gO_2 m^{-2} d^{-1}$] |
| $ksod$ | first-order kinetic constant [d^{-1}] |
| H | depth of the water column [m] |
| R_{sod} | sediment oxygen demand [$gO_2 m^{-3} d^{-1}$] |

V volume of the water compartment [m^3]

Positive DO

The concentration of dissolved oxygen (DO) may become negative in D-WAQ. 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 [$\text{gC m}^{-3} \text{ d}^{-1}$]

9.6 Suspended sediment, sedimentation and erosion

9.6.1 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 which can be classified according to the various grain sizes:

- | | |
|---------------------|-------------------------------|
| 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 μm |

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 principle 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 underwater light climate is an important environmental condition for algae growth. The presence of

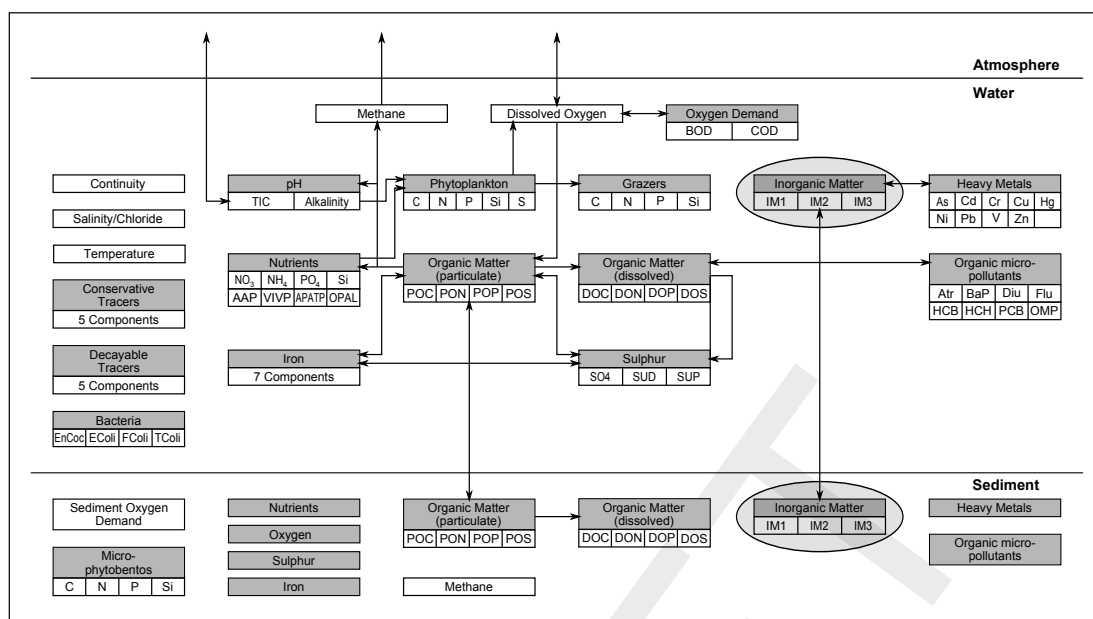


Figure 9.5: Overview of substances. Suspended sediment, sedimentation and erosion

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 is subject to settling in the water column and the fractions in the sediment are subject to erosion. The sediment can also be removed from the modelled part of the water system by burial. Remobilisation into the modelled system is possible by the reverse process indicated as 'digging'.

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-WAQ 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.

9.6.2 Modelling framework

The (inorganic) substances that can be modelled in the D-WAQ 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 \(9.9\)](#) and [Equation \(9.10\)](#) respectively.

$$\frac{\Delta c_w}{\Delta t} = \text{loads} + \text{transport} - \text{settling} + \text{resuspension} \quad (9.9)$$

$$\frac{\Delta c_b}{\Delta t} = \text{loads} + \text{settling} - \text{resuspension} - \text{burial} + \text{digging} \quad (9.10)$$

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. |
| 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. |
| 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. |

9.6.3 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](#)).

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 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.

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_e | 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-WAQ 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.

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.

$$\tau = \tau_{flow} + \tau_w + \tau_{ship} \quad (9.11)$$

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:

$$\tau_{flow} = \frac{\rho \cdot g}{C_{2D}^2} \cdot u^2 \quad \text{or} \quad \rho \cdot u_*^2 \quad (9.12)$$

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:

$$u(z) = \frac{u_*}{\kappa} \ln \left(\frac{z}{z_0} \right) \quad (9.13)$$

Averaging over the depth yields:

$$\bar{u} = \frac{u_*}{\kappa} \left[\ln \left(\frac{H}{z_0} \right) - 1 \right] \quad (9.14)$$

where:

$$u_* = \sqrt{g} \frac{\bar{u}}{C_{2D}} \quad (9.15)$$

Substitution of Equation (9.15) in Equation (9.14) results in an expression of z_0 :

$$z_0 = H e^{-\left(1 + \frac{\kappa \cdot C_{2D}}{\sqrt{g}}\right)} \quad (9.16)$$

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:

$$\tau_{flow} = \frac{g \rho_l}{C_{3D}^2} \vec{u}_b |\vec{u}_b| \quad (9.17)$$

$$C_{3D} = \frac{\sqrt{g}}{\kappa} \ln \left(1 + \frac{\Delta z_b / 2}{H} \right) \quad (9.18)$$

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 [$\text{m}^{-1/3} \text{s}^1$] |
| H | total water depth [m] |
| Δz_b | thickness of bed layer [m] |
| κ | constant of Von Kármán (0.4) [-] |
| k_s | Nikuradse roughness ($= 30z_0$) [m] |
| z_0 | roughness length (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 :

$$\text{water depth: } h_* = \frac{gh}{U_{10}^2} \quad (9.19)$$

$$\text{fetch: } F_* = \frac{gF}{U_{10}^2} \quad (9.20)$$

$$\text{wave height: } H_* = \frac{gH}{U_{10}^2} \quad (9.21)$$

$$\text{wave period: } T_* = \frac{gT}{U_{10}} \quad (9.22)$$

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

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

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-WAQ two commonly used formulations 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-WAQ 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:

$$D = w_s c$$



9.7 Nutrients, detrital organic matter and electron-acceptors

9.7.1 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-WAQ 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).

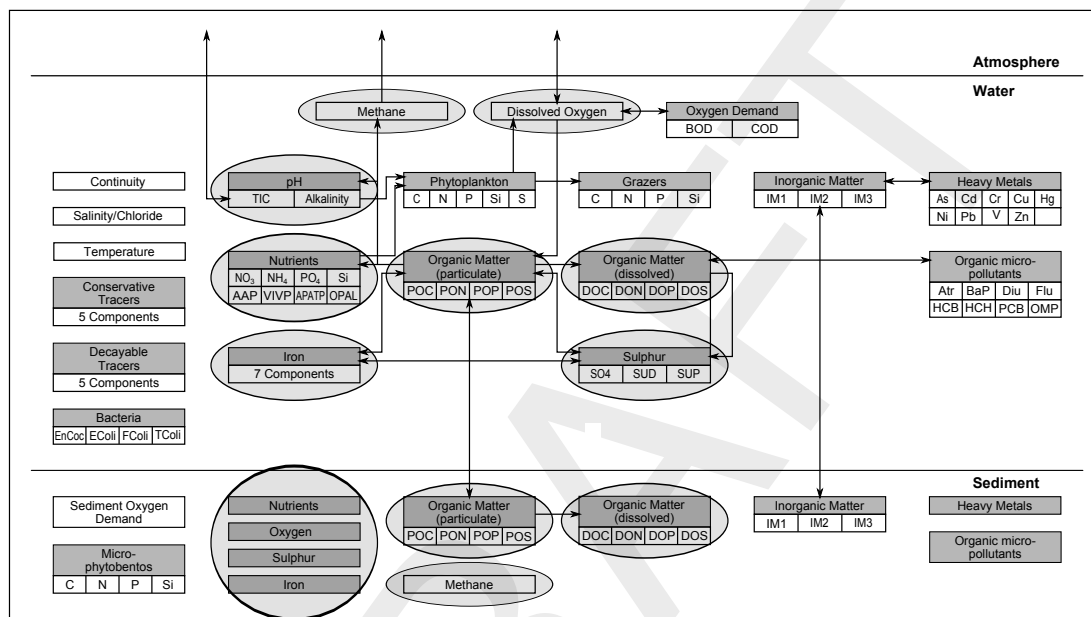


Figure 9.6: Overview of substances. Nutrients, detrital organic matter and electron-acceptors

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 9.8](#).

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.

9.7.2 Modelling framework

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

| Name of D-WAQ 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 |
| 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 |

⁵For a detailed description of sediment processes refer to [section 9.11](#).

| Name of substance | D-WAQ Description | Unit |
|---------------------------------------|---------------------------------|---------------------------------|
| 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 |
| CH ₄ | Methane | gC/m ³ |
| FeIIId | Dissolved Iron(III) | gFe/m ³ |
| FeIIlpa | Amorphous Iron (oxy)hydroxide | gFe/m ³ |
| FeIIlpc | Crystalline Iron (oxy)hydroxide | gFe/m ³ |
| FeIId | Dissolved Iron(II) | gFe/m ³ |
| FeS | Iron sulphide | gFe/m ³ |
| FeS ₂ | Pyrite | gFe/m ³ |
| FeCO ₃ | Iron carbonate | gFe/m ³ |

In present D-WAQ 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 (D-WAQ TRM, 2013)**.

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

umns are given in the equations below:

$$\frac{\Delta NO_3}{\Delta t} = \text{loads} + \text{transport} + \text{nitrification} - \text{denitrification} - \text{primary production} + \text{atmospheric deposition} \pm \text{sediment exchange flux} \quad (9.23)$$

$$\frac{\Delta NH_4}{\Delta t} = \text{loads} + \text{transport} - \text{nitrification} + \text{mineralization} - \text{primary production} + \text{autolysis} + \text{atmospheric deposition} \pm \text{sediment exchange flux} \quad (9.24)$$

$$\frac{\Delta PO_4}{\Delta t} = \text{loads} + \text{transport} \pm \text{sorption} + \text{mineralization} \pm \text{precipitation/dissolution} + \text{primary production} + \text{autolysis} + \text{atmospheric deposition} \pm \text{sediment exchange flux} \quad (9.25)$$

$$\frac{\Delta Si}{\Delta t} = \text{loads} + \text{transport} + \text{dissolution} - \text{primary production} + \text{autolysis} \pm \text{sediment exchange flux} \quad (9.26)$$

$$\frac{\Delta TIC}{\Delta t} = \text{loads} + \text{transport} + \text{mineralization} - \text{primary production} \pm \text{exchange atmosphere flux} \pm \text{sediment exchange flux} \quad (9.27)$$

$$\frac{\Delta SO_4}{\Delta t} = \text{loads} + \text{transport} + \text{sulphide oxidation} - \text{primary production} - \text{sulphate reduction} \pm \text{sediment return flux} \quad (9.28)$$

$$\frac{\Delta SUD}{\Delta t} = \text{loads} + \text{transport} + \text{sulphate reduction} - \text{sulphide oxidation} \pm \text{sediment return flux} \quad (9.29)$$

$$\frac{\Delta FeIIIpa}{\Delta t} = \text{loads} + \text{transport} \pm \text{precipitation-dissolution} - \text{iron reduction} - \text{settling} + \text{resuspension} \quad (9.30)$$

$$\frac{\Delta OM}{\Delta t} = \text{loads} + \text{transport} + \text{mortality} - \text{mineralization} - \text{grazing} - \text{settling} + \text{resuspension} \quad (9.31)$$

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 9.8](#).

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-WAQ. 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-WAQ.

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-WAQ are presented below.

| Process | Substances | Comments |
|------------------------|-------------------------------|--|
| Nitrification | NH4 NO3 (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 FeIIIpa (Alka) | $4Fe(OH)_3 + CH_2O \rightarrow 4FeII d + CO_2 + 2H_2O + 8OH^-$ <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 FeII (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 | FeIIIpa FeIIIpc 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-WAQ) |
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| Process | Substances | Comments |
|-----------------------------|---|--|
| Sediment ex- change flux | NO ₃ NH ₄ PO ₄ Si SO ₄ TIC OXY SUD CH ₄ FeIII FeII (Alka) | <ul style="list-style-type: none"> ◇ 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. ◇ 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). |
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| Process | Substances | Comments |
|------------------------|---|---|
| Mineralization | POC1-5 PON1-5 POP1-5 POS1-5 DOC DON DOP DOS NH4 PO4 SUD TIC (OXY) (NO3) (FeIIIpa) (FeIIId) (SO4) (CH4) (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 | NH4 PO4 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 FeIIId FeIIpa FeIIpc FeIId 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 FeIIpc and pyrite are produced from amorphous FeIIpa and FeS respectively. The aging of FeIIpa 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 CH ₄ | <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 FeS ₂ FeCO ₃ (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 9.6](#).

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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 $\text{g/m}^2/\text{d}$) 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. |
| Grazing | POC1-3 PON1-3 POP1-3 (Primary consumers) (Phytoplankton) (TIC) (OXY) (Alka) | <ul style="list-style-type: none"> ◇ Primary consumers can derive their nutrients from (living or death) organic matter. |
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| Process | Substances | Comments |
|----------------|-------------|---|
| pH equilibrium | TIC Alka | <ul style="list-style-type: none"> ◇ 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 9.3).
- ◇ Usually, the sediment is an essential pool of nutrients and organic matter. Refer to section 9.11.
- ◇ Ammonia (NH_3) and nitrite (NO_2^-) are not available as substances in D-WAQ. Both are already toxic at low concentrations, although concentrations are usually below the toxic levels. In D-WAQ 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.

**9.7.3 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 | rate of nitrification [$\text{gN m}^{-3} \text{d}^{-1}$] |
| 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 $\text{gFe}^{-1} \text{ m}^3 \text{ d}^{-1}$] |
| R_{ire} | rate of reduction [$\text{gFe m}^{-3} \text{ d}^{-1}$] |

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:

$$Kads = \frac{Cpha \times OH^a}{Cphd \times Cads}$$

$$Cadst = fcor \times \sum_{i=1}^3 (f_{Fe_i} \times Cimi) \times \frac{1}{56 \times 10^3 \times \varphi}$$

$$Rsorp = ksorp \times (Cphae - Cpha')$$

with:

| | |
|------------|---|
| a | stoichiometric reaction constant, equal to 0 for option 1 [-] |
| $Cads$ | free adsorbent concentration [mol Fe l _w ⁻¹] |
| $Cadst$ | total molar concentration of adsorption sites [mol Fe l _w ⁻¹] |
| $Cimi$ | concentration of inorganic matter fractions $i = 1, 2, 3$ [gDW m _ℓ ⁻³] |
| $Cpha$ | adsorbed phosphate concentration [moleP l _w ⁻¹] |
| $Cpha'$ | adsorbed phosphate concentration after the previous time-step [gP m _ℓ ⁻³] |
| $Cphae$ | equilibrium adsorbed phosphate concentration [mol P l _w ⁻¹] |
| $Cphd$ | dissolved phosphate concentration [mol P l _w ⁻¹] |
| $fcor$ | 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] |
| $ksorp$ | sorption reaction rate [d ⁻¹] |
| $Kads$ | adsorption equilibrium constant [mol ^{a-1} l ^{a-1}] |
| OH | adsorption equilibrium constant [mol l _w ⁻¹] |
| $Rsorp$ | rate of adsorption or desorption [gP m _ℓ ⁻³ d ⁻¹] |
| φ | porosity [-] |

With $fcor$ 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 $ksorp$. The equilibrium adsorbed phosphate concentration $Cphae$ can be calculated. The adsorption equilibrium constant $Kads$ 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 proportional 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 [$\text{gO}_2 \text{ m}^{-3}$] |
| 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 [$\text{m}^3 \text{w gO}_2^{-1} \text{ d}^{-1}$] |
| R_{prc} | rate of precipitation [$\text{gP m}^{-3} \text{ d}^{-1}$] |
| R_{sol} | rate of dissolution [$\text{gP m}^{-3} \text{ d}^{-1}$] |
| <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 [$\text{m}^3 \text{gSi}^{-1} \text{ d}^{-1}$] |
| R_{sol} | rate of opal silicate dissolution [$\text{gSi m}^{-3} \text{ d}^{-1}$] |
| 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}] |
|-----------|---|

| | |
|-------------|--|
| <i>IAP</i> | ion activity product [mol L ⁻¹] |
| <i>SOL</i> | solubility product [mol L ⁻¹] |
| <i>kprc</i> | precipitation reaction rate [gFe m ⁻³ d ⁻¹] |
| <i>kdis</i> | dissolution reaction rate [d ⁻¹] |
| <i>Rdis</i> | rate of dissolution [gFe m ⁻³ d ⁻¹] |
| <i>Rprc</i> | rate of precipitation [gFe m ⁻³ 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 FeIIlpa into FeIIlpc follows from:

$$Ra = ka \times CFea$$

with:

| | |
|-------------|---|
| <i>CFea</i> | concentration of amorphous FeIIlpa [gFe m ⁻³] |
| <i>ka</i> | aging reaction rate [d ₁] |
| <i>Ra</i> | rate of aging [gFe m ⁻³ d ⁻¹] |

The formation of pyrite follows from:

$$Ra = ka \times CFeS \times H2S$$

with:

| | |
|-------------|---|
| <i>CFeS</i> | concentration of FeS [gFe m ⁻³] |
| <i>H2S</i> | concentration of H2S [gS m ⁻³] |
| <i>kpyr</i> | formation of FeS2 [gS ⁻¹ m ³ d ₁] |
| <i>Rpyr</i> | rate of pyrite formation [gFe m ⁻³ 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:

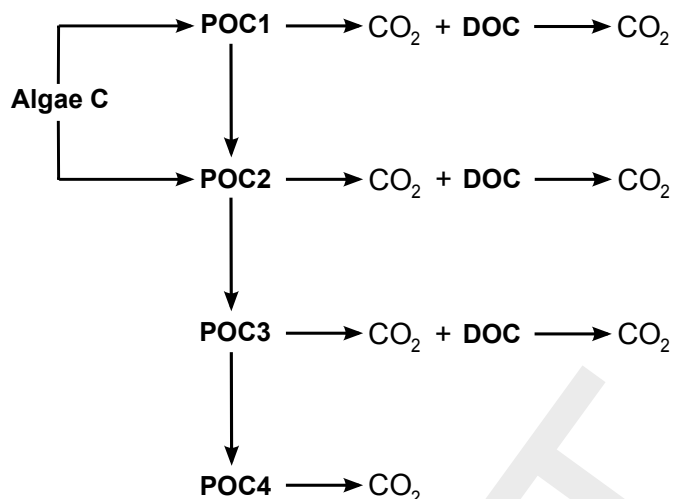
$$Rprc = 32\,000 \times kprc \times (Cs - Cse)$$

$$Rdis = 32\,000 \times kdis \times (Cse - Cs)$$

with:

| | |
|-------------|--|
| <i>Cs</i> | concentration of the free sulphide ion [mole L ⁻¹] |
| <i>Cse</i> | equilibrium concentration of the free sulphide ion [mole L ⁻¹] |
| <i>kprc</i> | precipitation reaction rate [d ⁻¹] |
| <i>kdis</i> | dissolution reaction rate [d ⁻¹] |
| <i>Rprc</i> | rate of precipitation [gS m ⁻³ d ⁻¹] |
| <i>Rdis</i> | rate of dissolution [gS m ⁻³ 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 9.5.3).

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.

9.8 Primary producers: phytoplankton

9.8.1 Concepts

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:

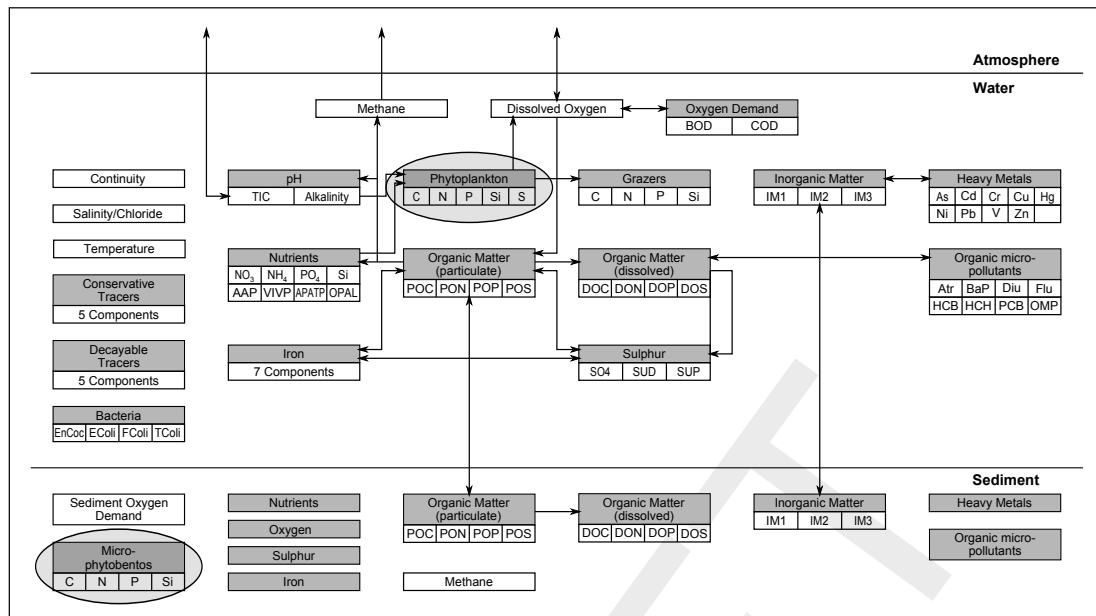


Figure 9.7: Overview of substances. Primary producers: phytoplankton

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 fixing 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.

9.8.2 Modelling framework

The substances that can be modelled in D-WAQ in relation to phytoplankton and microphyto-benthos are:

| Name of D-WAQ substance | Description | Unit |
|--------------------------------|--------------------|-------------------|
| <i>Phytoplankton: DYNAMO</i> | | |
| Diat | Diatoms | gC/m ³ |
| Green | Non-diatoms | gC/m ³ |
| <i>Phytoplankton: BLOOM</i> | | |

| Name of substance | D-WAQ | Description | Unit |
|----------------------------------|-------|--|-------------------|
| 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 |
| 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 9.7](#). [section 9.5](#) 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-WAQ.

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 fresh-water 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:

$$\frac{\Delta \text{Phytoplankton}}{\Delta t} = \text{loads} + \text{transport} - \text{settling} + \text{resuspension} + \text{gross primary production} - \text{respiration} - \text{mortality} \quad (9.32)$$

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 9.7](#)). 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-WAQ 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. |
| Respiration | All phytoplankton (NH ₄) (PO ₄) (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. |
| continued on next page | | |

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| Process | Substances | Comments |
|-------------------------|--|--|
| Mortality and autolysis | All phytoplankton POX1-2 (Opal) (NH ₄) (PO ₄) (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. |
| continued on next page | | |

⁷For a detailed description of the settling and resuspension process refer to [section 9.6](#).

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| Process | Substances | Comments |
|----------------------------|--|---|
| Resuspension ¹¹ | DiatS1 DiatS2 BLOOM algae (POX1-2) | <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. |
| 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 9.3](#) ($k = kr \times kt^{(T-Tr)}$). However, it is important to note that DYNAMO has a reference temperature of 20 °C, whereas BLOOM has a reference temperature of 0 °C.

9.8.3 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 9.9](#).

for nutrients,

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

for energy (light),

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

$$ecmin_i \leq eca \leq ecmax_i$$

$$ecmin_i = ectmin_i - ecb$$

$$ecmax_i = ectmax_i - ecb$$

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

$$Ia_i = f(Efc_i)$$

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>ecmax</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.

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

$$Rgp_i = Rgr_i + Rrsp_i + Rmrt_i$$

$$Rnp_i = Rgp_i - Rrsp_i$$

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

$$Raut_i = faut_i \times Rmrt_i$$

with:

| | |
|--------|---|
| $faut$ | 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:

$$Rgp_i = fnut_i \times flt_i \times kgp_i \times Calg_i$$

with:

| | |
|--------|---|
| $Calg$ | algal biomass concentration [gC m ⁻³] |
| flt | light limitation factor [-] |
| $fnut$ | nutrient limitation factor according to Monod [-] |
| kgp | potential gross primary production rate [d ⁻¹] |
| Rgp | 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:

$$fnut_i = \min \left(\frac{Cn}{Ksn + Cn}, \frac{Cph}{Ksph + Cph}, \frac{Csi}{Kssi + Csi} \right)$$

with:

| | |
|--------|--|
| Cn | ammonium plus nitrate concentration [gN m ⁻³] |
| Cph | phosphate concentration [gP m ⁻³] |
| Csi | dissolved inorganic silicate concentration [gSi m ⁻³] |
| Ksn | half saturation constant for nutrient nitrogen [gN m ⁻³] |
| $Ksph$ | half saturation constant for phosphate [gP m ⁻³] |
| $Kssi$ | 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:

$$flt_i = f(I_z, Io_i, DL, DLo_i, \dots)$$

with:

| | |
|-------|---|
| DL | day length [d] |
| DLo | optimal day length [d] |
| flt | light limitation factor [-] |
| I_z | depth average light intensity in a water layer [W m ⁻²] |
| Io | 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.

9.9 Primary consumption

9.9.1 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.

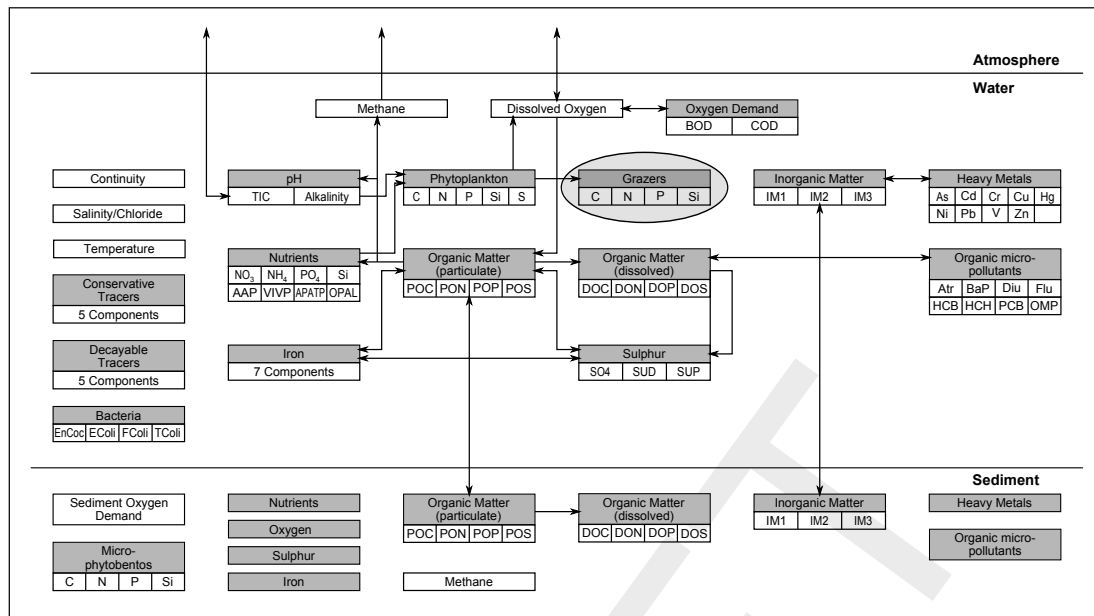


Figure 9.8: Overview of substances. Primary consumption

The modelling of all other processes to which the nutrients and detritus are subjected are described in [section 9.7](#) of this manual. [section 9.8](#) 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.

9.9.2 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 substance | D-WAQ | 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 |
| 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.

9.9.3 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 in stead 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 weigh 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 [-] |
| $fapr_{i,j}$ | 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:

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

with:

| | |
|-----------------|---|
| $f_{alg_{i,j}}$ | egested fraction of algae j consumed by grazer i , =1-yield [-] |
| f_{det_i} | egested fraction of detritus consumed by grazer i , =1-yield [-] |
| f_{sed_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.

9.10 Heavy metals and organic micro-pollutants

9.10.1 Concepts

Two types of micropollutants can be modelled with D-WAQ: heavy metals and organic micropollutants. 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-WAQ.

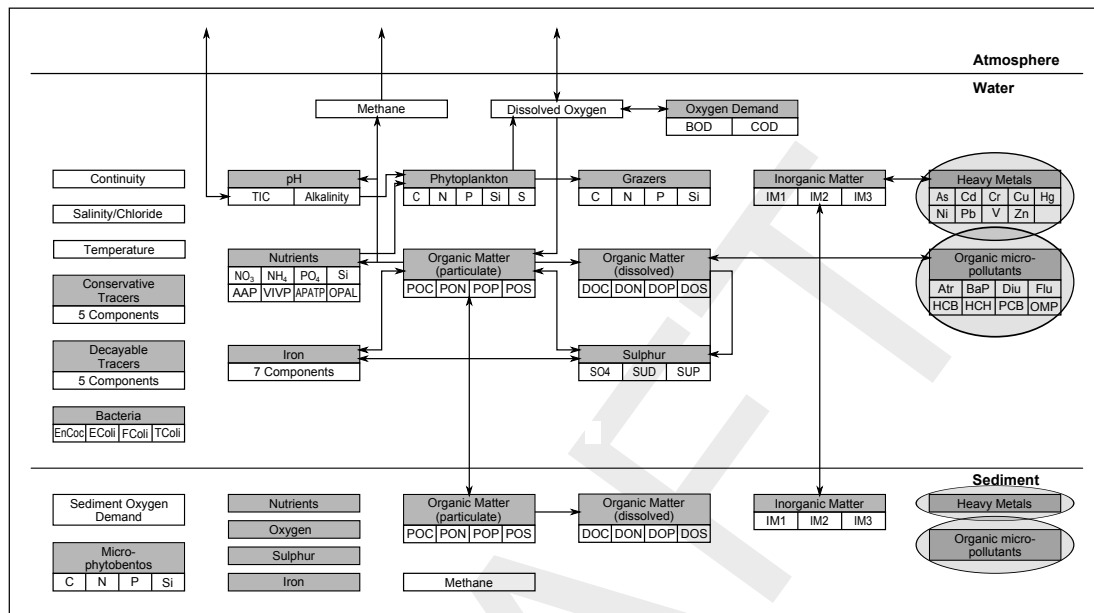


Figure 9.9: Overview of substances. Heavy metals and organic micro-pollutants

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-WAQ 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.

9.10.2 Modelling framework

Heavy metals

The heavy metals that can be modelled are divided among three subgroups:

| Name of D-WAQ substance | Description | Unit |
|--|-------------|------------------|
| <i>Group 1: sulphide-forming heavy metals</i> | | |
| Cd | Cadmium | g/m ³ |
| 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> | | |

| Name of substance | D-WAQ Description | Unit |
|--|-------------------|----------------|
| 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-WAQ uses one state variable (substance name) for equilibrium sorption, which represents the total metal concentration. Alternatively, D-WAQ 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 ($K_{pim_{1-3}}$, 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-WAQ allowing for joint simulation.

| Name of substance | D-WAQ Description | Unit |
|-------------------|-----------------------------------|------------------|
| OMP | (general) Organic Micro-Pollutant | g/m ³ |

| Name of substance | D-WAQ Description | Unit |
|-------------------|--|------------------|
| 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-WAQ 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-WAQ.
- 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).

9.10.3 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-WAQ 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:

$$Ct = (fim + fpoc + fdoc + falg + fd) \times Ct$$

$$fd = \frac{\phi}{\phi + Kpim \times Cim + Kppoc \times (Cpoc + Xdoc \times Cdoc) + Kpalg \times Calg}$$

$$fim = (1 - fd) \times \frac{Kpim \times Cim}{Kpim \times Cim + Kppoc \times (Cpoc + Xdoc \times Cdoc) + Kpalg \times Calg}$$

$$fpoc = (1 - fd) \times \frac{Kppoc \times Cpoc}{Kpim \times Cim + Kppoc \times (Cpoc + Xdoc \times Cdoc) + Kpalg \times Calg}$$

$$f_{doc} = (1 - f_d) \times \frac{X_{doc} \times K_{ppoc} \times C_{poc}}{K_{pim} \times C_{im} + K_{ppoc} \times (C_{poc} + X_{doc} \times C_{doc}) + K_{palg} \times C_{alg}}$$

$$f_{alg} = (1 - f_d - f_{im} - f_{poc} - f_{doc})$$

with:

| | |
|----------------------|---|
| $C_{alg/im/poc}$ | concentration of algae biomass [gC m ⁻³] inorganic matter, [gDW m ⁻³] dead particulate organic matter [gC m ⁻³] |
| C_t | total concentration of a micropollutant [mg m ⁻³] |
| $f_{alg/im/poc/doc}$ | fraction of a micropollutant adsorbed to algae biomass, inorganic matter, detrital particulate organic matter, dissolved organic matter [-] |
| f_d | dissolved fraction of a micropollutant [-] |
| $K_{palg/im/poc}$ | partition coefficient for algae [m ³ gC ⁻¹] inorganic matter [m ³ gDW ⁻¹] detrital particulate organic matter [m ³ gC ⁻¹] |
| X_{doc} | 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:

$$K_p = \frac{C_{p'}}{C_{d'}} = \frac{\phi \times C_p}{C_s \times C_d} \times 10^6$$

with:

| | |
|----------|---|
| K_p | equilibrium partition coefficient [mg.kg ⁻¹ DW/mg l ⁻¹ water] |
| $C_{d'}$ | dissolved concentration of a micropollutant [mg l ⁻¹ water] |
| $C_{p'}$ | particulate concentration of a micropollutant [mg.kg ⁻¹ DW] or [mg kg ⁻¹ C] |
| C_d | dissolved concentration of a micropollutant [mg m ⁻³] |
| C_p | particulate concentration of a micropollutant [mg m ⁻³] |
| C_s | 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:

$$R_{sorp} = k_{sorp} \times (C_{pe} - C_p)$$

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 [mg m ⁻³ 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-WAQ.

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-WAQ 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-WAQ. 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.

9.11 Sediment modelling

9.11.1 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 9.6](#). This section focuses on sediment diagenesis and the exchange of dissolved substances between the water column and the sediment.

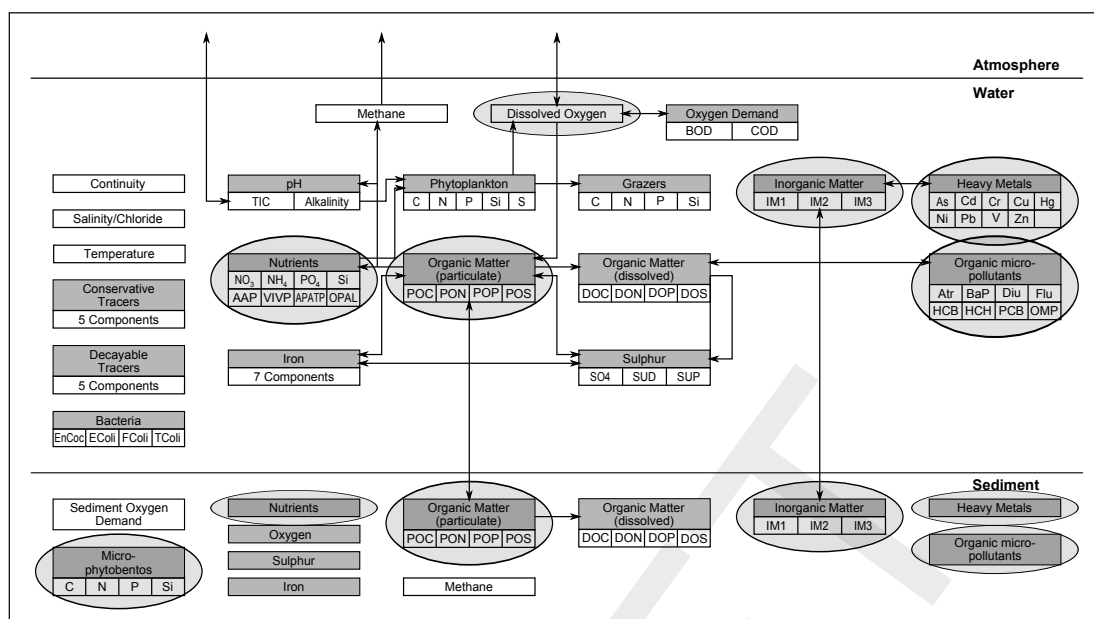


Figure 9.10: Overview of substances. Substances that are considered in the S1-S2 approach for sediment are encircled.

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 oxy-hydroxides (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 9.11](#) 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 9.11: 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 |
| 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.

9.11.2 Modelling framework

D-WAQ 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-WAQ, 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-WAQ:

| Name of substance | D-WAQ 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 |

| Name of substance | D-WAQ | Description | Unit |
|-------------------|-------|--|------|
| 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 9 for substances, processes and the dependency on chemical conditions.

9.11.3 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 9. 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 9.7. For phytoplankton see section 9.8. For primary consumers (grazers) see section 9.9. For heavy metals and organic micro-pollutants see section 9.10. For the inorganic matter fractions see section 9.6. 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 9.6. 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:

$$R_{loss} = \frac{k_{0_{loss}}}{H} + \frac{k_{loss} \times Cx}{V}$$

with:

| | |
|----------------|--|
| Cx | amount of a substance [gC/N/P/Si] |
| $k_{0_{loss}}$ | zero-order loss rate [$\text{g m}^{-2} \text{d}^{-1}$] |
| k_{loss} | first-order loss rate [d^{-1}] |
| R_{loss} | loss rate [$\text{gC/N/P/Si m}^{-3} \text{d}^{-1}$] |
| 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-WAQ 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.

9.12 Pre-defined sets, SOBEK only

9.12.1 Simple oxygen model (Streeter Phelps)

9.12.1.1 General

The Simple Oxygen Model is a so-called "pre-defined" set of selected state variables, active processes, editable input parameters and output parameters. It has been constructed with the Processes Library Configuration Tool. Experienced users may use the same tool to edit the predefined set.

9.12.1.2 State variables

The simple oxygen model distinguishes the following 3 state variables:

- ◇ dissolved oxygen (OXY);
- ◇ carbonaceous oxygen demand (CBOD5), represented by the 5 day value, expressed in gO_2/m^3 ;
- ◇ ammonium (NH_4), expressed in gN/m^3 , representing the nitrogenous oxygen demand.

9.12.1.3 Processes

The model equations for the state variables mentioned above include a number of processes from the Processes Library, which are described briefly below. For a formal description we refer to WAQ Technical Reference manual ([D-WAQ TRM, 2013](#)) for the individual processes of the Processes Library.

Carbonaceous BOD

The carbonaceous BOD is subject to a linear and temperature dependent *decay* process:

$$Flux = -k \times CBOD5 \times \theta^{T-20} \quad (9.33)$$

| | |
|----------|--|
| k | first order reaction rate (at 20 °C) [1/d] |
| θ | temperature dependency constant [–] |
| T | water temperature [°C] |
| $CBOD5$ | concentration of BOD ₅ [gO ₂ /m ³] |

The first order reaction rate (at 20 °C) is an input item. The temperature θ has a fixed value of 1.04. The oxygen consumption rate is computed automatically, taking into account the transformation of BOD₅ into ultimate bod.

The mineralisation is supposed to proceed at best under aerobic conditions. Therefore, the mineralisation process flux depends on the available amount of oxygen. If the oxygen concentration is over 5 mg/l, the process proceeds without limitation. If the oxygen concentration is below 1 mg/l, the process proceeds at 30 % of its unlimited rate. If the oxygen concentration is between 1 and 5 mg/l, the limitation factor varies linearly between 0.3 and 1.0. For details we refer to the BODCOD chapter in the WAQ Technical Reference manual ([D-WAQ TRM, 2013](#)).

Ammonium

The nitrification process removes ammonium. It is formulated linearly and temperature dependent:

$$Flux = -k \times NH_4 \times \theta^{T-20} \quad (9.34)$$

| | |
|----------|---|
| k | first order reaction rate (at 20 °C) [1/d] |
| θ | temperature dependency constant [–] |
| T | water temperature [°C] |
| NH_4 | concentration of NH ₄ (gN/m ³) |

The first order reaction rate (at 20 °C) is an input item. The temperature θ has a fixed value of 1.07. The mineralisation stops under a certain critical temperature, which is set to 3 °C. The oxygen consumption rate is computed as 4.571 times the nitrogen transformation rate, taking into account the proper chemical reaction formula and the molar weight of the participating components.

The nitrification process is supposed to proceed under aerobic conditions only. Therefore, the process flux depends on the available amount of oxygen. If the oxygen concentration is over 5 mg/l, the process proceeds without limitation. If the oxygen concentration is below 1 mg/l, the process stops completely. If the oxygen concentration is between 1 and 5 mg/l, the limitation factor varies linearly between 0 and 1. For details we refer to the NITRIF chapter in the WAQ Technical Reference manual ([D-WAQ TRM, 2013](#)).

Dissolved oxygen

Related to dissolved oxygen, some additional processes are included. The reaeration is formulated as a first order surface related process working on the oxygen deficit:

$$Flux = \frac{k}{H}(Oxy_{sat} - Oxy) \times \theta^{T-20} \quad (9.35)$$

| | |
|-------------|--|
| k | first order reaeration rate (at 20 °C) [m/d] |
| H | water depth [m] |
| θ | temperature dependency constant [–] |
| T | water temperature [°C] |
| Oxy | oxygen concentration [g/m ³] |
| Oxy_{sat} | saturation concentration [g/m ³] |

The first order reaeration rate in m/d is input to the model. The process is temperature dependent with the θ value equal to 1.016.

Additionally, there is a sediment oxygen demand process which allows the user to specify an autonomous oxygen consumption in g/(m²d). 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. For details we refer to the SEDOX chapter in the WAQ Technical Reference manual [D-WAQ TRM \(2013\)](#).

Note that the output dissolved oxygen concentration is made non-negative, while the modelled dissolved oxygen concentration can reach negative values if the consumption of oxygen is intensive enough. Such a negative concentration can be considered as more or less representing reduced substances.

9.12.1.4 Overview of all processes working on the state variables

| State variable | Processes acting on it |
|----------------|--|
| CBOD5 | Mineralisation BOD and COD |
| NH4 | Nitrification of ammonium |
| OXY | Mineralisation BOD and COD Nitrification of ammonium Reaeration of oxygen Sediment oxygen demand (additional) |

9.12.1.5 Overview of input items

The input parameters below can be specified through SOBEK's "Processes Library Coefficient Editor". A <*.plc> file with the recommended values is available, so that these values can be loaded (or reloaded) easily.

| Parameter id | Description | Recommended value | Unit |
|--------------|---|-------------------|----------|
| RcBOD | decay reaction rate BOD (first pool) at 20 °C | 0.7 | 1/d |
| RcNit | first-order nitrification rate constant | 0.1 | 1/d |
| KLRear | reaeration transfer coefficient | 1 | m/d |
| fSOD | zeroth-order oxygen demand flux | 6 | gO2/m2/d |

Additionally, the following items can be specified through the Meteorological Task.

| Parameter id | Description | Recommended value | Unit |
|--------------|-------------------|-------------------|------|
| Temp | Water temperature | n.a. | °C |

9.12.1.6 Output items

Apart from the concentrations of the state variables, the following parameters are available as extra output:

| Parameter id | Description | Unit |
|--------------|---|------|
| Depth | depth of segment | m |
| SaturOXY | saturation concentration | g/m3 |
| SatPercOXY | actual saturation percentage O2 | % |
| DO | non-negative dissolved oxygen concentration (defined as $\max(\text{OXY}, 0)$) | g/m3 |

9.12.2 Simple eutrophication model

9.12.2.1 General

The Simple Eutrophication Model is a so-called "pre-defined" set of selected state variables, active processes, editable input parameters and output parameters. It has been constructed with the Processes Library Configuration Tool. Experienced users may use the same tool to edit the predefined set.

9.12.2.2 State variables

The simple eutrophication model distinguishes the following 10 state variables:

- ◇ dissolved oxygen (OXY);
- ◇ inorganic nutrients: NH₄, NO₃, PO₄ (dissolved), AAP (adsorbed phosphates);
- ◇ inorganic suspended matter: IM1;
- ◇ algae ("Green");
- ◇ detritus: DetC, DetN, DetP.

9.12.2.3 Processes

The model equations for the state variables mentioned above include a number of processes from the Processes Library, which are described briefly below. For a formal description we refer to WAQ Technical Reference manual ([D-WAQ TRM, 2013](#)) for the individual processes of the Processes Library.

Suspended matter

The state variables representing suspended matter are subject to sedimentation. It concerns in particular IM1, AAP, DetC, DetN and DetP. The sedimentation process is formulated in terms of a settling velocity (input) and a sedimentation probability which depends on the local and momentaneous shear stress and a critical shear stress (input):

$$Flux = -V_{set} \left(1 - \frac{\tau}{\tau_{cr}} \right) \frac{C}{H} \quad (9.36)$$

| | |
|-------------|-----------------------------------|
| V_{set} | settling velocity [m/d] |
| τ | shear stress [N] |
| τ_{cr} | critical shear stress [N] |
| C | concentration [g/m ³] |
| H | water depth [m] |

See the SEDCAR chapter in the WAQ Technical Reference manual ([D-WAQ TRM, 2013](#)) for more details.

Resuspension is included only for inorganic suspended solids (IM1). It is formulated as a zero order flux (input) in g/(m²d).

The visual light extinction characteristics of the water are relevant for the growth of algae. The extinction depends on a background value (input) increased with a contribution of inorganic suspended matter, living algae and dead organic algae material (detritus):

$$E = E_{bg} + \sum_i e_i C_i \quad i \in \{\text{algae, detritus, inorganicsusp, solids}\} \quad (9.37)$$

| | |
|----------|---|
| E | light extinction [1/m] |
| E_{bg} | background light extinction [1/m] |
| e | specific extinction [m ² /g] |
| C | concentration [g/m ³] |

The specific extinction of each contribution to the extinction can be specified as input.

Algae-related processes

The simple eutrophication model includes a relatively simple model for the growth and mortality of algae. The growth process is formulated as a linear process, and can be expressed as follows:

$$\frac{\partial C}{\partial t} = \text{MaxGrowthRate} \times \text{NutrientLimitation} \times \text{LightLimitation} \times \text{DaylengthFactor} \times \text{TemperatureFactor} \times \text{ActualConcentration} \quad (9.38)$$

The Nutrient, Light and day length factors have a value between 0 and 1. The day length factor is defined as the quotient of the actual daylight period divided by an optimal value (input). The nutrient limitation factor is formulated as the product of two Monod type functions, one for N and one for P. The half saturation values are input items. The light limitation function is computed based on a linear extinction model and a "saturation value", which expresses the amount of light needed for optimal growth (input). The growth is *not reduced* when the light intensity exceeds the optimal value. The temperature factor is based on a θ type exponential function:

$$\text{temperature factor} = \theta^{T-20} \quad (9.39)$$

where

| | |
|----------|-------------------------------------|
| θ | temperature dependency constant [—] |
| T | water temperature [°C] |

The value of θ is input. For details we refer to the DLALG, NLALG, RADALG and TFALG chapters of the [D-WAQ TRM \(2013\)](#).

The growth is corrected for respiration, which is composed of a linear or "maintenance" part and a growth dependent part. The mortality of algae is again formulated as a linear process. Both respiration and mortality are temperature dependent. The value of J is input. For details we refer to the PRIPRO chapter of the WAQ Technical Reference manual ([D-WAQ TRM, 2013](#)).

The growth of algae causes an equivalent uptake of nutrients. To this end, the N-C-ratio and the P-C-ratio in living algae have to be specified as input. Similarly, the mortality of algae causes an equivalent release of nutrients. The release can be in organic form (detritus) or inorganic form, controlled by input parameters.

Mineralisation processes

The detritus is subject to a linear and temperature dependent mineralisation process:

$$\text{Flux} = -k \times C \times \phi^{T-20} \quad (9.40)$$

where

| | |
|--------|--|
| k | first order reaction rate (at 20 °C) [1/d] |
| ϕ | temperature dependency constant [—] |
| T | water temperature [°C] |
| C | concentration [g/m ³] |

The first order reaction rate (at 20 °C) as well as the temperature theta are input items. The mineralisation stops under a certain critical temperature, which is again input to the model.

Processes related to inorganic nutrients

Inorganic phosphorus occurs in two forms: dissolved (PO₄) and sorbed to inorganic suspended matter. The division over both forms is controlled by the adsorption process. A formulation according to Langmuir was selected. For details we refer to the ADSPO₄ chapter in the WAQ Technical Reference manual (D-WAQ TRM, 2013). The equilibrium constant is input to the model.

The nitrification process transforms ammonium into nitrates. It is formulated linearly and temperature dependent. The first order reaction rate (at 20 °C) as well as the temperature theta are input items. The mineralisation stops under a certain critical temperature, which is again input to the model. On top of this, also the oxygen concentration affects the nitrification rate. For details we refer to the NITRIF chapter in the WAQ Technical Reference manual (D-WAQ TRM, 2013).

The denitrification process effectively removes nitrates from the water column. It is formulated as a volumetric process, supposed to take place in the water column, when the oxygen concentration is low. It is formulated linearly and temperature dependent. The first order reaction rate (at 20 °C) as well as the temperature theta are input items. The process stops under a certain critical temperature, which is again input to the model. On top of this, also the oxygen concentration affects the denitrification rate. For details we refer to the DENWAT chapter in the WAQ Technical Reference manual (D-WAQ TRM, 2013).

Oxygen

Related to dissolved oxygen, some additional processes are included. The reaeration is formulated as a first order surface related process working on the oxygen deficit:

$$Flux = \frac{k}{H}(Oxy_{sat} - Oxy) \times \phi^{T-20} \quad (9.41)$$

where

| | |
|-------------|--|
| k | first order reaeration rate (at 20 °C) [m/d] |
| H | water depth [m] |
| ϕ | temperature dependency constant [—] |
| T | water temperature [°C] |
| Oxy | oxygen concentration [g/m ³] |
| Oxy_{sat} | saturation concentration [g/m ³] |

The first order reaeration rate in m/d is input to the model. The process is temperature dependent with the theta being an input parameter as well.

Additionally, there is a sediment oxygen demand process which allows the user to specify an autonomous oxygen consumption in g/(m²d). Note that the output dissolved oxygen concentration is made non-negative, while the modelled dissolved oxygen concentration can reach negative values if the consumption of oxygen is intensive enough. Such a negative concentration can be considered as more or less representing reduced substances.

Remaining processes

Additionally, the model includes a process to specify "diffuse loads" formulated as g/m²/d, for IM1, NH₄, PO₄, as well as auxiliary processes to compute the average water depth and the bottom shear stress from the geometric and hydraulic data passed to the water quality module by the channel flow module.

9.12.2.4 Overview of all processes working on the state variables

| State variable | Processes acting on it |
|------------------|---|
| OXY | Denitrification in water column Nitrification of ammonium Reaeration of oxygen Mineralisation detritus carbon Sediment oxygen demand (additional) Net primary production and mortality green algae |
| NH4 | Nitrification of ammonium Mineralisation detritus nitrogen Uptake of nutrients by growth of algae Release (nutrients/detritus) by mortality algae Diffusive waste NH4 |
| NO3 | Denitrification in water column Nitrification of ammonium Uptake of nutrients by growth of algae |
| PO4 | Ad(De)Sorption ortho phosphorus to inorg. Matter Mineralisation detritus phosphorus Uptake of nutrients by growth of algae Release (nutrients/detritus) by mortality algae Diffusive waste PO4 |
| AAP | Ad(De)Sorption ortho phosphorus to inorg. Matter Sedimentation AAP (adsorbed PO4) |
| IM1 | Sedimentation Resuspension Diffusive waste IM1 |
| Green | Net primary production and mortality green algae |
| DetC, DetN, DetP | Mineralisation detritus Release (nutrients/detritus) by mortality algae Sedimentation detritus carbon |

9.12.2.5 Overview of input items

The input parameters below can be specified through SOBEK's "Processes Library Coefficient Editor". A <*.plc> file with the recommended values is available, so that these values can be loaded (or reloaded) easily.

| Parameter id | Description | Recommended value | Unit |
|------------------------|---|-------------------|------|
| SWAdsP | switch formulation <0=Kd 1=Langmuir 2=GEM> | 1 | - |
| continued on next page | | | |

continued from previous page

| Parameter id | Description | Recommended value | Unit |
|------------------------|--|-------------------|---------------------|
| KdPO4AAP | partition coefficient PO4-AAP | 0.01 | m ³ /gDM |
| RcDenWat | first-order denit. rate constant water | 0.09 | 1/d |
| TcDenWat | temp. coefficient for denitrification | 1.045 | - |
| OOXDEN | optimum oxygen conc. for denitrification | 1 | g/m ³ |
| COXDEN | critical oxygen conc. for denitrification | 3 | g/m ³ |
| RcNit | first-order nitrification rate constant | 0.09 | 1/d |
| TcNit | temperature coefficient for nitrification | 1.08 | - |
| OOXNIT | optimum oxygen conc. for nitrification | 5 | g/m ³ |
| COXNIT | critical oxygen conc. for nitrification | 1 | g/m ³ |
| CTNit | critical temperature for nitrification | 3 | °C |
| RcDetN | first-order mineralisation rate constant | 0.18 | 1/d |
| TcDetN | temperature coefficient for mineralisation | 1.08 | - |
| CTMin | critical temperature for mineralisation | 3 | °C |
| RcDetP | first-order mineralisation rate constant | 0.18 | 1/d |
| TcDetP | temperature coefficient for mineralisation | 1.08 | - |
| NCRatGreen | Nitrogen-Carbon ratio in greens | 0.1 | gN/gC |
| PCRatGreen | Phosphorus-Carbon ratio in greens | 0.01 | gP/gC |
| FrAutGreen | frac. mort. greens dissolved as nutrients | 0 | - |
| FrDetGreen | frac. mort. greens to detritus | 1 | - |
| RcDetC | first-order mineralisation rate constant | 0.18 | 1/d |
| TcDetC | temperature coefficient for mineralisation | 1.08 | - |
| PPMaxGreen | maximum primary production green algae | 3 | 1/d |
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| Parameter id | Description | Recommended value | Unit |
|------------------------|--|-------------------|-------------------------|
| MRespGreen | maintenance respiration green algae | 0.03 | 1/d |
| GRespGreen | growth respiration factor green algae | 0.095 | - |
| Mort0Green | mortality rc of green algae st. temp | 0.2 | 1/d |
| VSedDetC | sedimentation velocity DetC | 0.5 | m/d |
| TauCSDetC | critical shear stress sedimentation DetC | 0.1 | N/m ² |
| VSedIM1 | sedimentation velocity IM1 | 1 | m/d |
| TaucSIM1 | critical shear stress sedimentation IM1 | 0.1 | N/m ² |
| fResS1DM | resuspension flux dry matter from S1 | 0 | gDM/(m ² d) |
| FrIM1S1 | fraction IM1 in sediment S1 | 1 | gDM/gDM |
| fDfWastIM1 | zeroth-order flux IM1 | 10 | gIM1/(m ² d) |
| fDfWastNH4 | zeroth-order flux NH4 | 0.05 | gNH4/(m ² d) |
| SWRear | switch for oxygen reaeration formulation <1–11> | 1 | - |
| KLRear | reaeration transfer coefficient | 1 | m/d |
| TCRear | reaeration temperature coefficient | 1.024 | - |
| Fsod | zeroth-order oxygen demand flux | 1 | gO2/(m ² d) |
| fDfWastPO4 | zeroth-order flux PO4 | 0.005 | gPO4/(m ² d) |
| ExtVIGreen | VI specific extinction Greens | 0.75 | m ² /gC |
| ExtVIDetC | VI specific extinction DetC | 0.47 | m ² /gC |
| ExtVIIM1 | VI specific extinction coefficient IM1 | 0.01 | m ² /gDM |
| ExtVIBak | background extinction visible light | 2 | 1/m |
| PrfNH4gree | ammonium preference over nitrate green algae | 1 | - |
| KMDINgreen | half-saturation value N green-algae | 0.025 | gN/m ³ |
| KMPgreen | half-saturation value P green-algae | 0.005 | gP/m ³ |
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| Parameter id | Description | Recommended value | Unit |
|--------------|---|-------------------|------------------|
| Cl | Chloride concentration | 200 | g/m ³ |
| TcGroGreen | temp. coeff. for growth processes green algae | 1.06 | - |
| TcDecGreen | temp. coeff. for resp./mort. green algae | 1.045 | - |
| DayL | day length <0-1> | 0.58 | d |
| OptDLGreen | day length for growth saturation green-algae | 0.58 | d |
| RadSatGree | total radiation growth saturation greens | 80 | W/m ² |

Additionally, the following items can be specified through the Meteorological Task.

| Parameter id | Description | Recommended value | Unit |
|--------------|--------------------------------------|-------------------|------------------|
| Temp | Water temperature | n.a. | °C |
| Rad | Solar radiation at the water surface | n.a. | W/m ² |

DRAFT

10 Numerical aspects

10.1 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 (Delft3D-FLOW UM, 2013). 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 10.1). 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.

$$T_y = \int_{y_l}^{y_r} \frac{\partial}{\partial y} \left(D \frac{\partial C}{\partial y} - v_y C \right) dy = \left(D \frac{\partial C}{\partial y} - v_y C \right) \Big|_{y=y_l}^{y=y_r} = 0 \quad (10.1)$$

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 10.1) occurs the 'stock terms' at the right hand side of Equation (10.1) 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:

$$\frac{\partial}{\partial t}(A\bar{C}) = \frac{\partial}{\partial x} \left(D \frac{\partial A\bar{C}}{\partial x} \right) - \frac{\partial}{\partial x} \int_y \int_z (v_x C) dy dz + A\bar{f}(\bar{C}, \dots, t) + AS \quad (10.2)$$

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 (10.2) there is one term which will be discussed in more detail here.



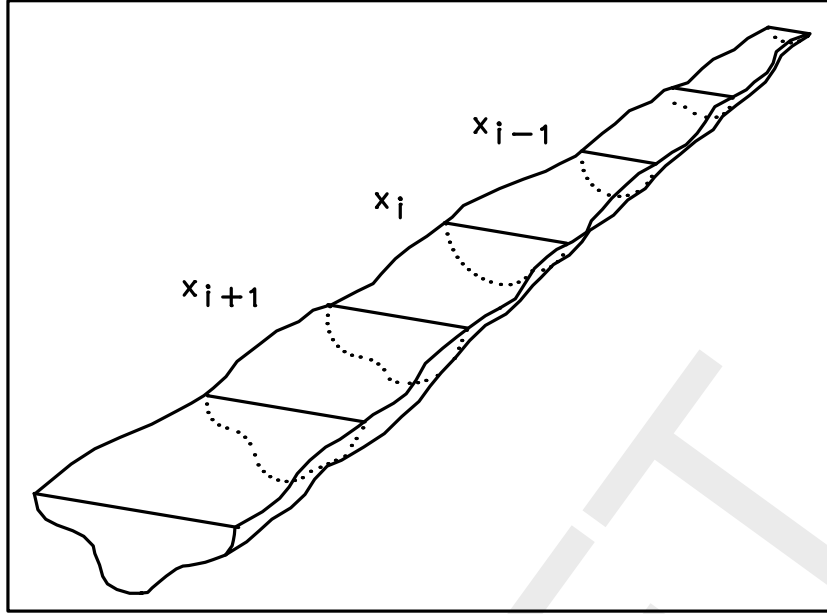


Figure 10.1: Estuary represented as a 1-dimensional model

With:

$$v_x = \bar{v}_x + \Delta v_x \quad \text{and} \quad C_x = \bar{C}_x + \Delta C_x, \quad (10.3)$$

the advective term of Equation (10.2) is:

$$\frac{\partial}{\partial x} \int_y \int_z (v_x C) dy dz = \frac{\partial}{\partial x} (\bar{v}_x A \bar{C}_x) + \frac{\partial}{\partial x} \int_y \int_z (\Delta v_x \Delta C_x) dy dz \quad (10.4)$$

If Δv_x and ΔC_x (which are functions of y and z) are not correlated at all, the last term of Equation (10.4) 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 10.2).

A well known approximation is, that this transport is proportional to the concentration difference over the small turbulence distance:

$$T_{add} = -\frac{\partial}{\partial x} \int_y \int_z (\Delta v_x \Delta C_x) dy dz \approx -\Delta v_x \Delta x_t \frac{(C_{x+\Delta x_t} - C_x)}{\Delta x_t} \approx -K \frac{\partial C}{\partial x} \quad (10.5)$$

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 (10.5) 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

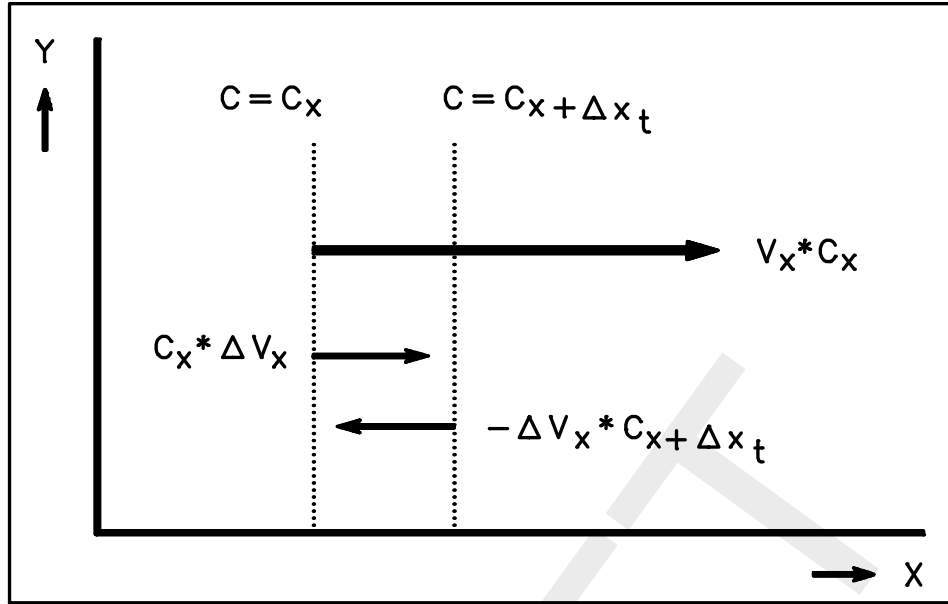


Figure 10.2: Effect of turbulent fluctuations Δv_x on the net transport

integration is performed over the whole cross-sectional area of a small estuary instead of only over the scale of turbulences.

Figure 10.3 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 10.3. 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 (10.5) 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 turbulence

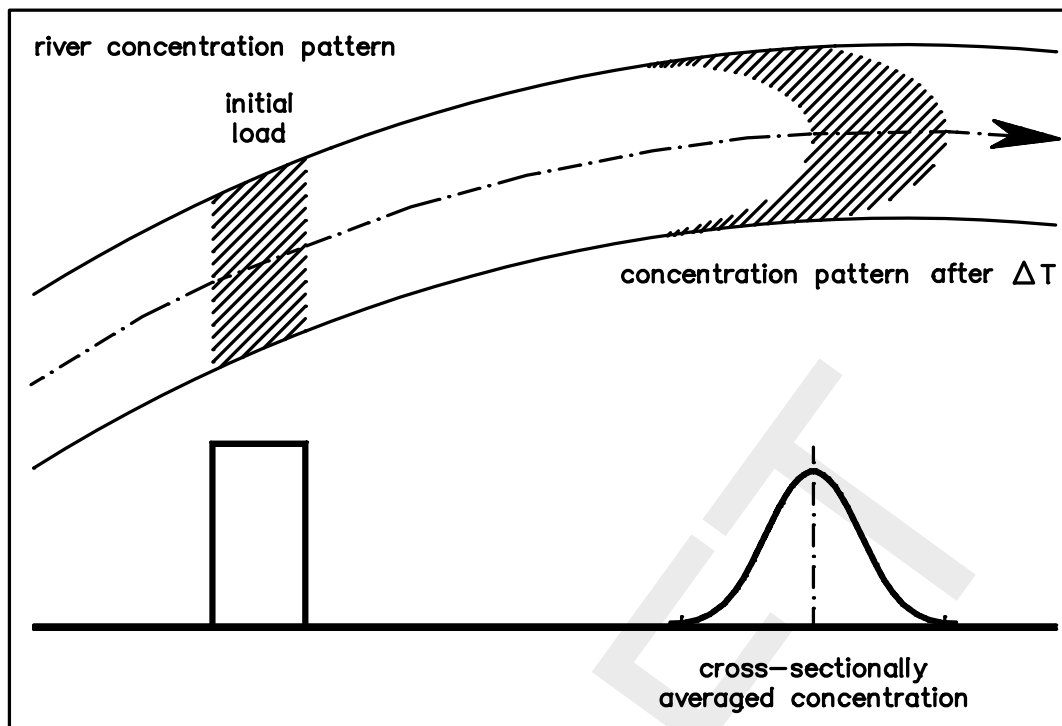


Figure 10.3: "Dispersion" by inhomogeneity of flow in a cross-sectionally averaged one-dimensional model

models (incorporated in Delft3D-FLOW) 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 10.1](#) 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 Delft3D-FLOW's turbulence model.

Table 10.1: 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 |

10.2 Introduction to algorithmic implementation

The multi-dimensional water quality program D-WAQ 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-WAQ for the advection-diffusion-reaction equation. A lot of different integration schemes are available in D-WAQ. 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-WAQ will be addressed in this chapter.

10.3 Conceptual description

10.3.1 Partial differential equations

The advection-diffusion-reaction equation in D-WAQ reads:

$$\frac{\partial C}{\partial t} = -\vec{u} \cdot \vec{\nabla} C + \vec{\nabla} \cdot (\vec{D} \cdot \vec{\nabla} C) + S + f_R(c, t) \quad (10.6)$$

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:

$$f_r(c, t) = -kc \quad (10.7)$$

For incompressible flow the conservation law of mass, also known as volume balance, is given by:

$$\vec{\nabla} u = 0 \quad (10.8)$$

The volume balance is computed by Delft3D-FLOW, which is Deltares program 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.

10.3.2 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 (10.6) over the computational cells, and subsequently applying Gauss' divergence theorem:

Gauss' theorem:

$$\int_V \vec{\nabla} \cdot \vec{W} dV = \oint_A \vec{W} \cdot \vec{n} dA \quad (10.9)$$

with \vec{W} an arbitrary vector. The resulting equations are the following integro-differential equations:

ADVECTION-DIFFUSION IN FLUX-FORM:

$$\frac{dM}{dt} + \oint_A (\vec{u}C) \cdot \vec{n} dA = \oint_A (\vec{D} \cdot \vec{\nabla} C) \cdot \vec{n} dA \quad (10.10)$$

CONTINUITY EQUATION:

$$\frac{dV}{dt} + \oint_A \vec{u} \cdot \vec{n} dA = 0 \quad (10.11)$$

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:

$$\bar{C} = \frac{M}{V} \quad (10.12)$$

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:

$$\oint_A (\vec{u}C) \cdot \vec{n} dA = \sum_{j=1,n} \int_{A_{i \rightarrow j}} (\vec{u}C) \cdot \vec{n} dA \approx \sum_{j=1,n} (Q \cdot \tilde{C})_{i \rightarrow j} \quad (10.13)$$

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:

$$\frac{d(V\bar{C})_i}{dt} + \sum_{j=1,n} (Q\tilde{C})_{i \rightarrow j} = \sum_{j=1,n} \left(D \frac{\partial \tilde{C}}{\partial x} \right)_{i \rightarrow j} A_{i \rightarrow j} \quad (10.14)$$

Flows and volumes in this equation follow from Delft3D-FLOW. Also exchange faces A can be derived from Delft3D-FLOW. 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:

$$\frac{dV_i}{dt} = \sum_{j=1,n} Q_{i \rightarrow j} \quad (10.15)$$

This equation can also be derived by substituting a constant number (constant water density) for concentrations in Equation (10.13).

10.4 Numerical discretisation

10.4.1 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:

$$\frac{d(V\bar{C})_i}{dt} = - \sum_{j=1,n} (Q\tilde{C})_{i \rightarrow j} + \sum_{j=1,n} \left(D \frac{\partial \tilde{C}}{\partial x} \right)_{i \rightarrow j} A_{i \rightarrow j} + f_R(\bar{C}_i, t) + S_i \quad (10.16)$$

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

10.4.2 Time discretisation and stability criteria

Time-discretisation is explicit, implicit or semi-implicit. Consider the equation in form:

$$\frac{\partial c}{\partial t} = Lc \quad (10.17)$$

with:

L = differential operator

The general recipe for time-discretisation for D-WAQ is:

$$\frac{c_{t+\Delta t} - c_t}{\Delta t} + \text{H.O.T.} = (1 - \theta)(Lc)_t + \theta(Lc)_{t+\Delta t} \quad (10.18)$$

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-WAQ expand the time-derivative at the right hand side to second order. Third order terms are not (yet) included in D-WAQ 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-WAQ the 'Courant-Friedrichs-Lewy' (CFL) condition for stability is:

$$\Delta t < \frac{V_i}{\sum_{j=1,n} Q_{i \rightarrow j}} \quad (10.19)$$

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:

$$\Delta t < \frac{1}{\left(\frac{2 \sum D_{xx}(A_{yz_{i \rightarrow j}}/V_i)}{\Delta x_i} + \frac{2 \sum D_{yy}(A_{xz_{i \rightarrow j}}/V_i)}{\Delta y_i} + \frac{2 \sum D_{zz}(A_{xy_{i \rightarrow j}}/V_i)}{\Delta z_i} + \frac{\sum_i Q_{i \rightarrow j}}{V_i} \right)} \quad (10.20)$$

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-WAQ has such schemes. In D-WAQ 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-WAQ. 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-WAQ, so one must take care if the time step of the computation is not short vis-a-vis the time scales of the input.

10.4.3 Discretisation of transport and numerical diffusion

This section explains the numerical schemes of D-WAQ. D-WAQ calculates mass derivatives (in time) of:

- 1 advective transport
- 2 diffusive transport
- 3 reaction terms

4 source terms

D-WAQ uses the following scheme in order to proceed one step in time:

$$\Delta M_i^{t+\Delta t} = \Delta M_i^t + \Delta t \left(\frac{\Delta M}{\Delta t} \right)_{Tr} + \Delta t \left(\frac{\Delta M}{\Delta t} \right)_R + \Delta t \left(\frac{\Delta M}{\Delta t} \right)_S \quad (10.21)$$

$$C_i^{t+\Delta t} = \frac{M_i^{t+\Delta t}}{V_i^{t+\Delta t}} \quad (10.22)$$

$$\begin{aligned} \left(\frac{\Delta M}{\Delta t} \right)_{Tr} &= \text{mass derivative of advective and diffusive transport} \\ \left(\frac{\Delta M}{\Delta t} \right)_R &= \text{mass derivative of reactions} \\ \left(\frac{\Delta M}{\Delta t} \right)_S &= \text{mass derivative of sources} \end{aligned}$$

All numerical schemes in D-WAQ (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*:

$$C^{t+\Delta t} = C^t + \Delta t \left(\frac{\partial C}{\partial t} \right)_t \quad (10.23)$$

and

$$\left(\frac{\partial C}{\partial t} \right)_t = f(C^t, FF^t, MP) \quad (10.24)$$

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:

$$\Delta t < \frac{1}{2|k|} \quad (10.25)$$

Thus, the quicker the process (higher value of k), the smaller the allowed time step.

For dispersive transport, concentration gradients in D-WAQ always follow from a *central discretisation*:

$$\frac{\partial \tilde{C}}{\partial x} \approx \frac{\bar{C}_j - \bar{C}_i}{\Delta x_{i \rightarrow j}} \quad (10.26)$$

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-WAQ, with centrally discretised gradients for diffusion, and with a θ -splitting in time is:

$$\begin{aligned} \frac{M_i^{t+\Delta t} - M_i^t}{\Delta t} + \dots \text{ (H.O.T.)} &= (1 - \theta) \left[- \sum_{j=1,n} (Q\tilde{C})_{i \rightarrow j} + \sum_{j=1,n} D_{i \rightarrow j} \frac{\bar{C}_j - \bar{C}_i}{\Delta x} A_{i \rightarrow j} \right]^t \\ &+ (\theta) \left[- \sum_{j=1,n} (Q\tilde{C})_{i \rightarrow j} + \sum_{j=1,n} D_{i \rightarrow j} \frac{\bar{C}_j - \bar{C}_i}{\Delta x} A_{i \rightarrow j} \right]^{t+\Delta t} + \left(\frac{\Delta M}{\Delta t} \right)_R^t + \left(\frac{\Delta M}{\Delta t} \right)_S^t \end{aligned} \quad (10.27)$$

The schemes of D-WAQ 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.

10.5 Numerical schemes in D-WAQ

First, we will summarise the numerical schemes in D-WAQ briefly. The subsequent sections provide detailed information for each numerical scheme.

Overview of numerical schemes in D-WAQ

Numerical schemes

- ◇ Schemes 1 to 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 should only be used in special cases
- ◇ Scheme 10:
 - As scheme 1 but implicit
 - Uses a direct inversion of the matrix to find the solution at $t + \Delta t$
 - Can be applied in 3D simulations, but direct inversion may be very time consuming
- ◇ 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:
 - Schemes are also used in Delft3D-FLOW
 - ADI (Alternating Direction Implicit) used
 - Aggregation of the hydrodynamic database is not allowed
 - Remove inactive cells is also not allowed
 - Very accurate, but iterative solver may require small time step to comply with accuracy criterion
- ◇ 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

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 19/20 → most accurate, but computation time may be long and grid aggregation or 'active only' coupling not allowed
- 2 Scheme 12 (3D) or scheme 5 (2D) → accurate, but must fulfil stability criterion
- 3 Scheme 21/22 → fast but accuracy dependent on time step, no stability criterion
- 4a. Scheme 1 → less accurate than scheme 5, but more robust (larger time step)
- 4b. Scheme 15/16 → Generally very fast scheme, but numerical dispersion may be large
- 4c. Scheme 10 → only 2D, less accurate than scheme 5, but no stability criterion

10.5.1 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:

$$\tilde{C}_{i \rightarrow j} = \begin{cases} \bar{C}_i & \text{for } Q_{i \rightarrow j} > 0 \\ \bar{C}_j & \text{for } Q_{i \rightarrow j} < 0 \end{cases} \quad (10.28)$$

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:

$$\frac{M_i^{t+\Delta t} - M_i^t}{\Delta t} = \left[- \sum_{j=1,n}^{\text{outflowing}} Q_{i \rightarrow j} \bar{C}_i - \sum_{j=1,n}^{\text{inflowing}} Q_{i \rightarrow j} \bar{C}_j + \sum_{j=1,n} D_{i \rightarrow j} \frac{(\bar{C}_j - \bar{C}_i)}{\Delta x} A_{i \rightarrow j} \right]^t + \left(\frac{\Delta M}{\Delta t} \right)_R^t + \left(\frac{\Delta M}{\Delta t} \right)_S^t \quad (10.29)$$

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:

$$D_{num} = \frac{1}{2}(u\Delta x - u^2\Delta t) \quad (10.30)$$

$$\text{E.g.: } u = 0.1 \text{ m/s, } \Delta x = 1000 \text{ m, } \Delta t = 0.5 \text{ h} \Rightarrow D_{num} = 41 \text{ m}^2/\text{s}$$

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.).

10.5.2 Second order Runge-Kutta (Scheme 2)

This scheme uses $\theta = 0$ (explicit) for time. However, the scheme uses a *predictor-corrector* method (see below) for calculation of the time derivative, including *transport derivatives*, *source terms* and *reaction derivatives*. Therefore, the method is second order accurate in time. It is the only method in D-WAQ that discretises the reaction terms with higher order accuracy. Apart from this, all characteristics for scheme 1 are also valid for this method. For a double time step the method is as efficient as scheme 1.

(or *predictor-corrector scheme*):

predictor:

$$\frac{c_{t+\Delta t/2} - c_t}{\Delta t/2} = (Lc)_t \quad (10.31)$$

corrector:

$$\frac{c_{t+\Delta t} - c_t}{\Delta t} = (Lc)_{t+\Delta t/2}$$

The operator L includes all processes, e.g. transport and all (including non-linear) water-quality processes. By using the two step predictor-corrector method, these processes are now more accurate in time. The use of this scheme is limited since in water-quality modelling most concentration changes due to processes are relatively slow compared those due to transport, and thus can be described well by first order schemes. Thus the time step requirements are more stringent for transport.

10.5.3 Lax Wendroff method (Scheme 3)

This method is second order in time (H.O.T.'s are included) and in space. The face averaged concentration follows from a *central discretisation*:

$$\tilde{C}_{i \rightarrow j} = \frac{\bar{C}_i + \bar{C}_j}{2} \quad (10.32)$$

The method is explicit, it uses $\theta = 0$.

$$\begin{aligned} & \frac{M_i^{t+\Delta t} - M_i^t}{\Delta t} \\ &= \left[- \sum_{j=1,n} Q_{i \rightarrow j} \left(\frac{\bar{C}_i + \bar{C}_j}{2} \right) + \sum_{j=1,n} Q_{i \rightarrow j}^2 \Delta t \frac{(\bar{C}_j - \bar{C}_i)}{A_{i \rightarrow j} \Delta x} + \sum_{j=1,n} D_{i \rightarrow j} \frac{(\bar{C}_j - \bar{C}_i)}{\Delta x} A_{i \rightarrow j} \right]^t \\ &+ \left(\frac{\Delta M}{\Delta t} \right)_R^t + \left(\frac{\Delta M}{\Delta t} \right)_S^t \end{aligned} \quad (10.33)$$

Note that this method can not deal with exchange faces A that are zero. The interfacing module of Delft3D is safeguarded by setting A to 1.0 m^2 in such a case.

The method is:

- ◇ 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 problems.

- ◇ not positive. Spurious oscillations and negative concentrations occur at steep concentration fronts.
- ◇ conditionally stable, according to the CFL condition.
- ◇ accurate to second order.

10.5.4 Alternating Direction Implicit (2D) method (Scheme 4)

This method is second order in time and space, and uses a $\theta = 0.5$ (semi-implicit) scheme. The method is unconditionally stable. The method can be applied for 1D systems (it is then known as the Crank-Nicolson method) and 2D-systems for *structured* grids (see Chapter 5) only. The method can not be applied for 3D models. Integration schemes 19 and 20 represent ADI methods that are suitable for 3D models.

With respect to the space discretisation, method 4 is identical to method 3. Thus, central discretisations are applied. Owing to its semi-implicit time integration *i* no stability criteria are required. However, oscillations may occur. The method becomes less accurate when large time steps are used, especially in case of irregular model boundaries.

10.5.5 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 Delft3D 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.

10.5.6 Scheme 6

Not available in D-WAQ.

10.5.7 Scheme 7

Not available in D-WAQ.

10.5.8 Scheme 8

Not available in D-WAQ.

10.5.9 Scheme 9

Not available in D-WAQ.

10.5.10 Implicit Upwind scheme with a direct solver (Scheme 10)

This method is like method 1 but it uses $\theta = 1.0$ (fully implicit) for time discretisation. The following linear system of equations must be solved:

$$\begin{aligned} \frac{V_i^{t+\Delta t} \bar{C}_i^{t+\Delta t}}{\Delta t} + \left[\sum_{j=1,n}^{\text{outflowing}} Q_{i \rightarrow j} \bar{C}_i + \sum_{j=1,n}^{\text{inflowing}} Q_{i \rightarrow j} \bar{C}_j + \sum_{j=1,n} D_{i \rightarrow j} \frac{\bar{C}_i - \bar{C}_j}{\Delta x_{i \rightarrow j}} A_{i \rightarrow j} \right]^{t+\Delta t} \\ = \frac{M_i^t}{\Delta t} + \left(\frac{\Delta M_i}{\Delta t} \right)_R^t + \left(\frac{\Delta M_i}{\Delta t} \right)_S^t \end{aligned} \quad (10.34)$$

In matrix-notation this equation reads

$$\vec{A} \cdot \vec{c} = \vec{b} \quad (10.35)$$

where

| | |
|-----------|----------------------|
| A | matrix |
| \vec{c} | concentration vector |
| \vec{b} | 'load vector' |

Note: that the diagonal entries of the matrix are always positive.



These diagonal entries of A are given by:

$$A_{ii} = \frac{V_i^{t+\Delta t}}{\Delta t} + \left[\sum_{j=1,n}^{\text{outflowing}} Q_{i \rightarrow j} + \sum_{j=1,n} D_{i \rightarrow j} \frac{A_{i \rightarrow j}}{\Delta x_{i \rightarrow j}} \right]^{t+\Delta t} \quad (10.36)$$

Here summation is only over flows that are flowing out of the segment. Note that these entries never can get zero (even when all flows are flowing in), or negative. This ensures unconditional numerical stability. Getting the concentrations at $t + \Delta t$ requires the solution of this system of linear equations. Methods to solve this equation are 'direct methods' or iterative solvers. For scheme 10, D-WAQ uses a direct method. The method is a lower-, diagonal-, upper-matrix (LDU) decomposition with gauss-elimination (Golub and Van Loan, 1989). LDU decomposition always renders answers, however, the method may be very CPU expensive and/or may require huge amounts of hard core computer memory (although the implementation in D-WAQ was optimised for efficiency). The costs of the method, and the amount of computer memory required depend on the bandwidth of matrix A. The bandwidth

is given by the number of diagonals and co-diagonals in A that have at least one entry that is not equal to zero. This costs follows the number of co-diagonals p and the dimension of the matrix n according to $\frac{1}{2}np^2$ (Golub and Van Loan, 1989), i.e. a number raised to the third power. For 3D systems the method can not be used due to unfeasible large CPU costs (p will be very large then). In such a case iterative solvers (methods 15 and 16) must be used.

An advantage of the method is that when transport for some (say N) substances is exactly equal (when Q and D are equal for these substances), the cost for getting N solutions is nearly equal to the cost of one solution. Thus for simulations with hundreds of substances that all have equal transport this method may be very efficient. The method is:

- ◇ computationally demanding, especially for most 3D problems;
- ◇ For simulations with hundreds of substances that all have equal transport the method may be very efficient (but not in 3D);
- ◇ positive
- ◇ there are no stability criteria for transport. Therefore larger times-steps may be used;
- ◇ first order accurate, the second order error is known as *numerical dispersion* (see scheme 1).
- ◇ Very large time steps will lead to loss of accuracy.

Note that this method also works for extremely (or infinite) time-steps in case no reaction terms are present. In such a case, the so-called steady state solution of the advection-diffusion equation is obtained. However, for large time-steps reaction terms may start to put stability requirements on the solution since these are still treated explicitly.

10.5.11 Horizontal Upwind scheme, Vertical: implicit in time and central discretisation (Scheme 11)

Method 10 is not feasible for most 3D models. However, the use of explicit schemes in 3D modelling is not advised since stability criteria are, in general, very stringent for vertical diffusive transport. Therefore, implicit schemes should be applied for vertical transport. They need not be applied for horizontal transport since stability criteria here lead to workable time-steps. Since mass fluxes can be divided in fluxes for horizontal and vertical direction in D-WAQ (i.e. transport within layers, and transport between the layers) D-WAQ can solve these equations independently. In such a case, all equations in vertical direction reduce to simple 1-dimensional systems over the layers. In vertical direction scheme 4 (Crank-Nicolson method) is used.

Method 11 also 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.

10.5.12 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 is less efficient than scheme 11.
- ◇ Not positive. Spurious oscillations and negative concentrations may occur for stratified systems.
- ◇ Conditionally 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.

10.5.13 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.*

10.5.14 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.*

10.5.15 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, 1994a, 1996a). This implies that the system of equations is transformed to a system that can be solved more easily:

$$M^{-1}A \vec{c} = M^{-1} \vec{b} \quad (10.37)$$

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-WAQ 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.

10.5.16 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.

10.5.17 Scheme 17

Not available in D-WAQ.

10.5.18 Scheme 18

Not available in D-WAQ.

10.5.19 ADI scheme for 3D models (horizontal: higher order scheme, vertical: central discretisation (Scheme 19))

Scheme 4 in D-WAQ represents an ADI-type scheme that is only suitable for 1D or 2D models. It makes use of central spatial differences, see [section 7.1.4.4](#). Scheme 19 is an ADI-type scheme that is identical to the scheme used in Delft3D-FLOW for the solution of (conservative) transport processes. Similarly to scheme 4, scheme 19 can only be applied to structured grids (aggregation of the hydrodynamic file not allowed).

The ADI methods consists of two stages. At one stage a central discretisation is applied (see [Equation \(10.32\)](#)), whereas at the other stage a higher order upwind method is used:

$$\tilde{C}_{i \rightarrow j} = \begin{cases} \frac{10\bar{C}_i - 5\bar{C}_{i-1} + \bar{C}_{i-2}}{6} & \text{for } Q_{i \rightarrow j} > 0 \\ \frac{10\bar{C}_j - 5\bar{C}_{j+1} + \bar{C}_{j+2}}{6} & \text{for } Q_{i \rightarrow j} < 0 \end{cases} \quad (10.38)$$

We remark that owing to the structured grid we have that $j = i + 1$. Discretisation of [Equation \(10.38\)](#) also requires information at two grid cells away. If such information is not available, for example near boundaries, dry points and constructions, the discretisation in [Equation \(10.38\)](#) is simplified to (if possible [Equation \(10.39a\)](#) is applied, otherwise [Equa-](#)

tion (10.39b))

$$\tilde{C}_{i \rightarrow j} = \frac{3\bar{C}_i - \bar{C}_{i-1}}{2} \quad \text{for } Q_{i \rightarrow j} > 0 \text{ and } \bar{C}_{i-2} \text{ not available} \quad (10.39a)$$

$$\tilde{C}_{i \rightarrow j} = \bar{C}_i \quad \text{for } Q_{i \rightarrow j} > 0 \text{ and } \bar{C}_{i-1} \text{ not available} \quad (10.39b)$$

For $Q_{i \rightarrow j} < 0$ a similar simplification is applied. In the vertical direction the central discretisation Equation (10.32) is applied.

This scheme is

- ◇ very accurate and also able to simulate sharp gradients.
- ◇ unconditionally stable. Thus, large time steps can be applied.
- ◇ not positive. Spurious oscillations and (small) under- and overshoots may occur at steep fronts, see remark below.
- ◇ only available for structured grids.

It is known that Eulerian mesh computations with second or higher order advective difference methods exhibit non-physical oscillations near steep gradient regions of the solution. Consequently negative concentrations may occur. This is the case for scheme 19 as well. Thus, positive solutions are not guaranteed. However, in case of negative concentrations an iterative procedure based on local diffusion may be started in order to smooth out negative values. A non-linear smoothing operator is applied with removes the negative concentrations c.q. computational noise, without inflicting significant accuracy losses in sharply peaked solutions. This smoothing technique is the so-called Forester filter (Forester, 1979).



Remark:

- ◇ When the 1 domain WAQ model originates from a multi-domain FLOW simulation, scheme 19 cannot be used.

10.5.20 ADI scheme for 3D models (horizontal: higher order scheme, vertical: upwind discretisation (Scheme 20))

Owing to the central discretisation in the vertical for scheme 19, oscillations may occur in the computations. Therefore, scheme 20 has been made available in D-WAQ that uses the same discretisations in the horizontal direction, but an upwind discretisation in the vertical direction. As a result, no oscillations are generated because of the discretisation in the vertical direction. However, the numerical solution is more diffusive compared to the one of scheme 19.



Remark:

- ◇ When the 1 domain WAQ model originates from a multi-domain FLOW simulation, scheme 20 cannot be used.

10.5.21 Local-theta flux-corrected transport scheme (Scheme 21 and 22)

Scheme 5 in D-WAQ 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 pro-

cessing 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. \(2009\)](#).

10.6 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](#)) and ([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:

$$x = x^*, y = y^*, \sigma = \frac{z - \zeta}{H} \quad (10.40)$$

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:

$$\frac{\partial^2 c}{\partial x^2} = \frac{\partial^2 c^*}{\partial x^{*2}} + \left(\frac{\partial \sigma}{\partial x} \right)^2 - \frac{\partial^2 c^*}{\partial \sigma^2} + 2 \frac{\partial \sigma}{\partial x} - \frac{\partial^2 c^*}{\partial x^* \partial \sigma} + \frac{\partial^2 \sigma}{\partial x^2} - \frac{\partial c^*}{\partial \sigma}. \quad (10.41)$$

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, 1985](#)) 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 ([Delft3D-FLOW UM, 2013](#)).

If the same approach is used for the horizontal diffusion operator in the transport equation:

$$\frac{\partial^2 c}{\partial x^2} \approx \frac{\partial^2 c^*}{\partial x^{*2}}, \quad (10.42)$$

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.

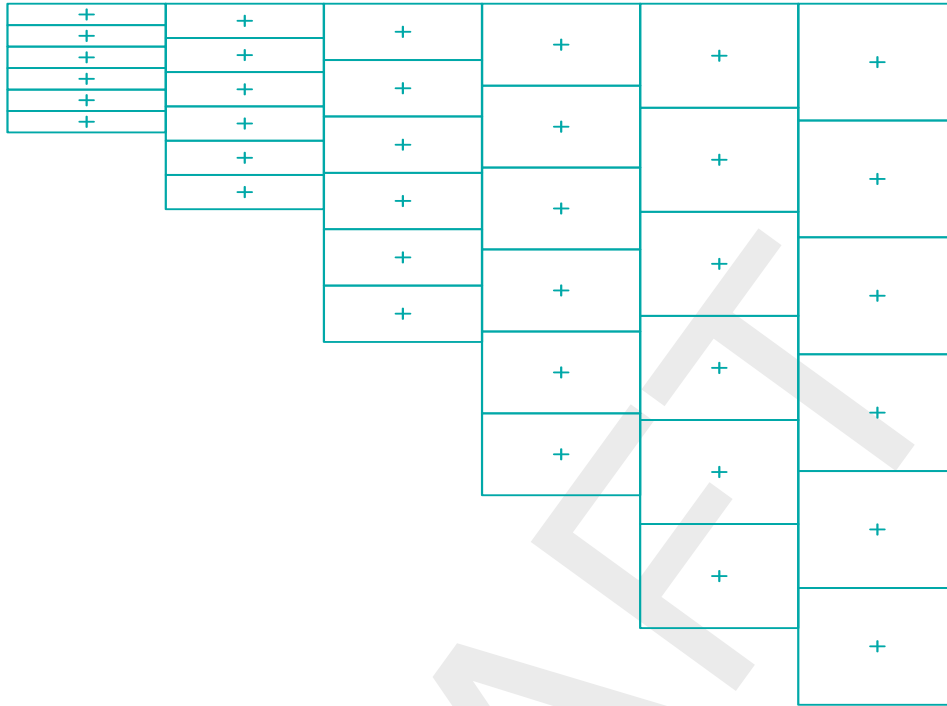


Figure 10.4: Finite Volume for diffusive fluxes and pressure gradients

Like in Delft3D-FLOW, in D-WAQ an option is available that minimises artificial vertical diffusion due to truncation errors; see [section 5.3.9: Numerical options](#). 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 10.4](#). 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 10.5](#), 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 10.5](#). [Stelling and Van Kester \(1994\)](#) apply a non-linear filter to combine the two consistent approximations of the horizontal gradient, $s_1 = \frac{c_2^* - c_1}{\Delta x}$ and $s_2 = \frac{c_2 - c_1^*}{\Delta x}$:

$$\text{If } s_1 \times s_2 < 0 \text{ Then} \quad (10.43)$$

$$\frac{\Delta c}{\Delta x} = 0$$

Else

$$\frac{\Delta c}{\Delta x} = \text{sign}(s_1) \times \min(|s_1|, |s_2|)$$

Endif

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

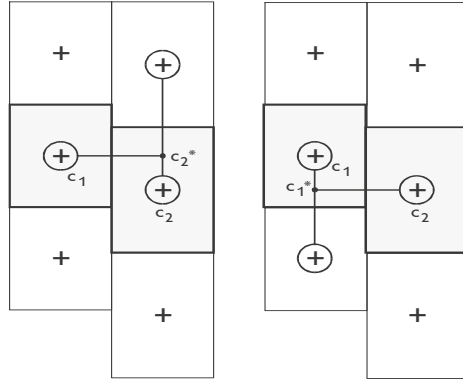


Figure 10.5: Left and right approximation of a strict horizontal gradient

integration of the horizontal diffusion term is explicit with time step limitation:

$$\Delta t \leq \frac{1}{D_H} \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right)^{-1}. \quad (10.44)$$

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-WAQ is both

consistent and assures the min-max principle:

$$\begin{aligned} &\text{If } s_1 \times s_2 < 0 \quad \text{Then} \\ &\quad \frac{\Delta c}{\Delta x} = 0 \\ &\text{Elseif } |s_4| < |s_3| \quad \text{Then} \\ &\quad \frac{\Delta c}{\Delta x} = s_4 \\ &\text{Elseif } \min(|s_1|, |s_2|) < |s_3| < \max(|s_1|, |s_2|) \quad \text{Then} \\ &\quad \frac{\Delta c}{\Delta x} = s_3 \\ &\text{Else} \\ &\quad \frac{\Delta c}{\Delta x} = \text{sign}(s_1) \min(|s_1|, |s_2|) \\ &\text{Endif} \end{aligned} \tag{10.45}$$

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.

11 Special features

11.1 Built-in coupling with Delft3D-FLOW

Often the communication files resulting from computations with a large hydrodynamic model (or over a long simulation period) are very large and mostly exclusively used for the coupling to other modules, such as D-Water Quality. This means that disk space is not used efficiently, unless you have reasons to experiment with the parameters of the coupling process, such as aggregating in time or space.

If the conversion to the files used by the water quality modules is fixed, then it is possible to write directly the hydrodynamic quantities to file, these files can be used by D-Water Quality without the need of any intermediate program. This option is called built-in coupling with D-Water Quality and can be switched on in the FLOW-GUI (Delft3D-FLOW UM, 2013) data group *Output* → *Storage* by tick off the check box *Export WAQ input*, see Figure 11.1.

The screenshot shows the 'Storage' tab in the FLOW-GUI. It contains two main sections: 'FLOW simulation times' and 'Store map results'. The 'FLOW simulation times' section has fields for 'Start time' (05 08 1990 00 00 00), 'Stop time' (06 08 1990 01 00 00), and 'Time Step [min]:' (5). The 'Store map results' section has fields for 'Start time' (05 08 1990 00 00 00), 'Stop time' (06 08 1990 01 00 00), and 'Interval' (120 [min]). There is also a 'History interval' field (10 [min]). To the right, the 'Store communication file' section has fields for 'Start time' (05 08 1990 12 30 00), 'Stop time' (06 08 1990 01 00 00), and 'Interval' (30 [min]). At the bottom, there are checkboxes for 'Fourier analysis' (unchecked), 'Online visualisation' (unchecked), and 'Export WAQ input' (checked). There is a 'Select file' button and a text field 'File : Filename unknown'. An 'Edit WAQ input >>' button is also present.

Figure 11.1: Data Group Output → Storage to switch on Export WAQ input

Remark:

- ◇ The option *Online coupling* is not available any more.



11.2 Domain decomposition

The current implementation of domain decomposition in Delft3D-FLOW means that for each domain separate communication files are created. To avoid having to select all these files separately and to specify the various parameters (start and stop time for instance) in a way that is consistent for all domains, you simply select the <*.ddb> file belonging to the computation as a whole, instead of a communication file.

This file describes how the various domains are connected. It is created automatically while you define the multiple domains and the corresponding hydrodynamic input. The user-interface

for the coupling program then reads the information contained in this file, so that it can prepare the conversion of the communication files per domain.

The only locations where you as a user are confronted with the fact that multiple domains are involved are:

- ◇ The selection of a <*.ddb> file, instead of a communication file.
- ◇ Associating aggregation files (from D-Waq DIDO) with individual domains.

The latter is due to the fact that currently D-Waq DIDO can not handle multiple domains. Instead you have to specify the spatial aggregation per domain.

11.3 Online coupling between Delft3D-FLOW and SOBEK

In some cases it is advantageous to model a part of the area of interest with a one-dimensional flow model (like for instance SOBEK) and another part with a multidimensional model. For instance, if you have a complicated network of rivers and channels that flow into an estuary and then into the open sea. Modelling such a system with a multidimensional model only can force you into using a very large detailed grid, just because of the need to include all branches of the network.

An alternative is to use two simultaneously running computations that interact. While the technical details of this set-up are quite complex, they are of no particular importance to the use of such a system. What is important is that this can be done and how it can be done.

The communication (or “online coupling”) between the two computations involves a simple convention: the names of the boundaries between the two regions must match. That is: if the one-dimensional model has a boundary “River”, for which the connection with the multidimensional model must be established, then this name must appear in the list of boundaries for the multidimensional model. This is the strategy for the hydrodynamic models and it is the strategy for the water-quality models as well.

The user-interface can assist here:

- ◇ The hydrodynamic description file can be expanded to hold information about these special boundaries.
- ◇ These boundaries become “reserved” in the sense that you can not change the name or the location of these boundaries (otherwise the communication would go wrong).
- ◇ If the two models are run simultaneously, so that data can be passed to and from, any boundary concentrations you put into the scenario for these boundaries will be ignored. However, it is still possible to edit the boundary data, as you may wish to run the multidimensional model standalone.
- ◇ If you run the multidimensional model standalone, there is only one minor limitation: the concentration data for such boundaries are *always* uniform over the whole section, but the *same input files can be used for both types of computation*. As such boundary sections are generally short, this is but a minor limitation.

The boundary section designated for the communication are specified as follows in the hyd-file:

```
boundaries-coupled-externally
  'Name'   xbegin  ybegin  xend  yend
  ... repeated for each such boundary section ...
end-boundaries-coupled-externally
```


where:

- ◇ 'Name' is the identification of the boundary in question (the string used to recognise the boundary in both computations).
- ◇ *xbegin* and *ybegin* the indices of the start of the boundary section
- ◇ *xend* and *yend* the indices of the end of the boundary section

11.4 Converting results of a hydrodynamic model using Z -model

The hydrodynamic module in Delft3D can handle both so-called σ -model and z -model (see [Delft3D-FLOW UM \(2013\)](#)). The latter require a different conversion program, as the concept is quite different. For the user, however, this should be almost completely transparent. This section describes the way z -layers are handled in the water quality module.

There is one important aspect to z -layers that differs from σ -layers: the treatment of active segments:

- ◇ In a model using σ -layers all segments in the same column are either active or inactive, depending on the water level. In the water quality module, a threshold is used for most water quality processes to make sure that in very shallow segments (typically segments that are dry or are almost dry) the processes that depend on the thickness of the water layer remain bounded. When the segments are dry, the flow over the interfaces is zero, so that also the dispersion is turned off.
- ◇ In a model using z -layers on the other hand, the topmost segment can become dry, whereas the segments below it still hold water. At a later time the topmost segment can get wet again or the segment below it can become dry in turn as well. To take care of this dynamics, a special "water quality process" monitors the thickness of the water layer and sets the attribute for the segment to *inactive* once the thickness is below a certain threshold or to *active* if it is above the threshold again. In this way, completely analogous to what happens in the hydrodynamic module, the drying and flooding of segments in a z -layer model is handled¹.

As the hydrodynamic database itself does not allow for a reliable detection of the type of layers that has been used, the hydrodynamic description file has been extended with two new keywords, σ -layers and z -layers that can be added after the keyword *geometry*:

The following lines both define a curvilinear grid with σ -layers (this being the default type of layers):

```
geometry curvilinear-grid
geometry curvilinear-grid sigma-layers
```

To define z -layers, you need to explicitly add the keyword *z-layers*:

```
geometry curvilinear-grid z-layers
```

The effect is that in the water quality computation the process *Emersion* is turned on with the specific parameter $Z_{threshold}$ that determines if the water layer is thick enough for the segment to be active or not. *Note*: this is taken care of automatically by the user-interface.

¹As all the regular water quality processes are implemented to deal with active and inactive segments, the z -layer feature is completely transparent to the water quality module in all other respects.

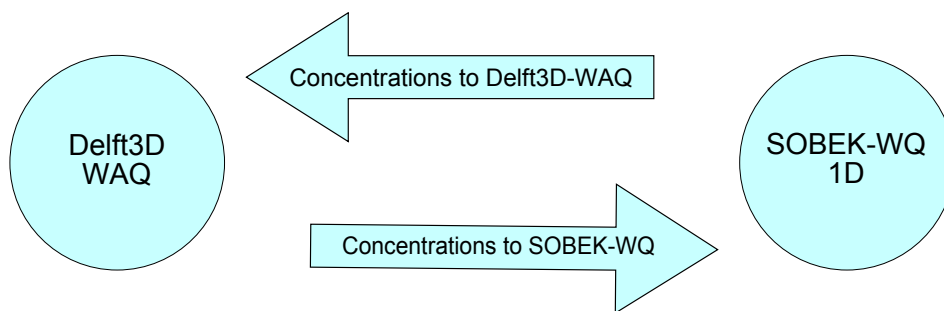


Figure 11.2: Approach for coupling of 3D and 1D model.

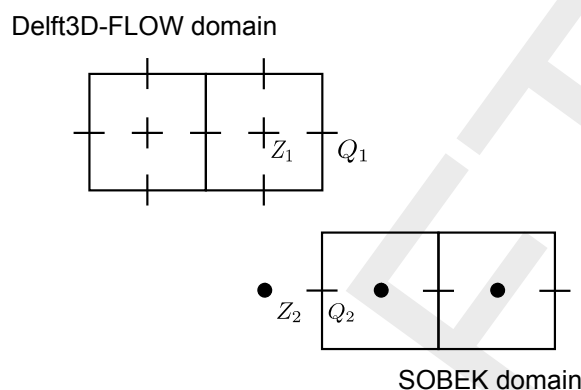


Figure 11.3: Illustration of coupling of D-WAQ and SOBEK-WQ 1D model.

11.5 1D–3D Coupling

11.5.1 Mathematical background

The Deltares System is able to perform joint (on-line coupled) simulations for one 1D domain, modelled within the 1D software suite SOBEK, and one 3D domain, modelled within the Delft3D suite. Both systems simulate time dependent processes for which a time stepping procedure is applied.

In the coupled 1D–3D model the concentrations of the state variables are exchanged between both domains at each time step. A so-called explicit coupling is applied. This means that model quantities are exchanged between the 1D part and the 3D part and that the data from the other part is stored as input variable of the equations. At every time step, the 1D domain sends the concentration values in the cells adjacent to the coupling boundary, to the 3D domain as its boundary conditions, and vice versa. This is illustrated in [Figure 11.2](#).

The 1D and 3D domains optionally use an implicit time integration method, which requires the solution of a system of equations. For reasons of flexibility, we chose not to apply an implicit coupling approach. An implicit coupling would require the solving of one large system of equations, which integrates the systems of equations of the 1D and 3D model domains. Instead, the explicit approach described above was selected.

The boxes, [Figure 11.3](#), show the control volumes used for setting up the water quality model in both domains, relative to the water level points (Z_i) and velocity points in both domains (Q_i). It is evident that the control volumes in both domains are correctly aligned and allow for a mass conserving solution.

The implementation of the 1D–3D coupling is such that one SOBEK grid cell corresponds to

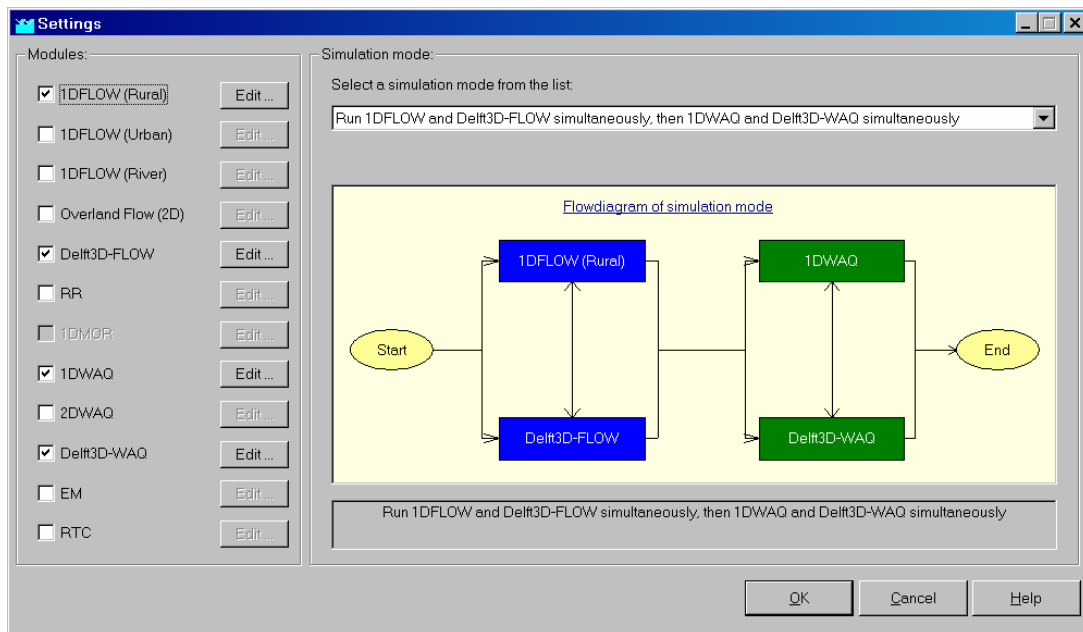


Figure 11.4: Overview of activated modules.

one open boundary segment in Delft3D-FLOW. If this open boundary segment consists of n computational cells, each of k vertical layers, then the concentrations of the 1D segment are transferred as boundary conditions to all nk 3D segments, while the concentrations from all nk 3D segments are used as boundary conditions for the 1D segment. In the latter case, the value transferred is the flow-weighted average concentration. It should be noted that it is common to use an upwind spatial discretisation on the model boundaries. In that case only the boundary conditions from the “upwind” domain affect the “downwind” domain. The transfer of boundary conditions from the downwind to the upwind domain is done for administrative reasons only. Evidently, the definition of “upwind” depends on the local and momentaneous direction of flow.

The coupling as it is implemented does not allow for a different time step in the coupled domains: the same time step should be used in the 1D and 3D domains. In practice, 1D simulations usually run with a larger time step than 3D simulations. Therefore, the time step synchronisation of the domains means that the time step in the 1D domain is probably smaller than it would have been in stand alone mode. This will evidently not hamper the accuracy of the calculations. Since the performance of the joined 1D–3D model is, to a large extent, determined by the 3D domain, the overall performance is not significantly affected by the synchronisation.

The fact that the coupling is implemented in an explicit fashion implies that the selection of an explicit solution method of the governing equations is required to guarantee conservation of mass. It is not expected however that the use of implicit methods will cause significant errors. This expectation has been confirmed by test simulations during practical applications.

11.5.2 Software implementation

In general the input for both domains is arranged via the respective User Interfaces of SOBEK (1D domain) and Delft3D (3D domain). The simulation is started from the SOBEK User Interface. To activate this mode of calculation, activate the *Settings* task in the SOBEK User Interface, and make the selection as shown in [Figure 11.4](#).

After a successful simulation, the inspection of the output is again arranged via the respective User Interfaces of SOBEK (1D domain) and Delft3D (3D domain).

The facilities to carry out coupled 1D–3D simulations are available from versions 3.28.06 of Delft3D and 2.12 of SOBEK.

11.5.3 Tutorial

For making a successful combined 1D–3D water quality simulation, the following requirements need to be met:

- ◇ A valid 1D–3D coupled hydrodynamic simulation needs to be available (we refer to the related Manual).
- ◇ This hydrodynamic simulation needs to have produced the necessary output files for a joint water quality simulation (see [section 11.5.3.1](#)).
- ◇ Other input necessary for the 1D and 3D domains of the water quality model needs to have been prepared (see [section 11.5.3.2](#)).

The on-line connection the 1D and 3D domain can then be arranged as described in [section 11.5.3.3](#). This section also describes how boundaries, time steps and state variables will be matched between both domains.

11.5.3.1 Hydrodynamic input files for the water quality simulation

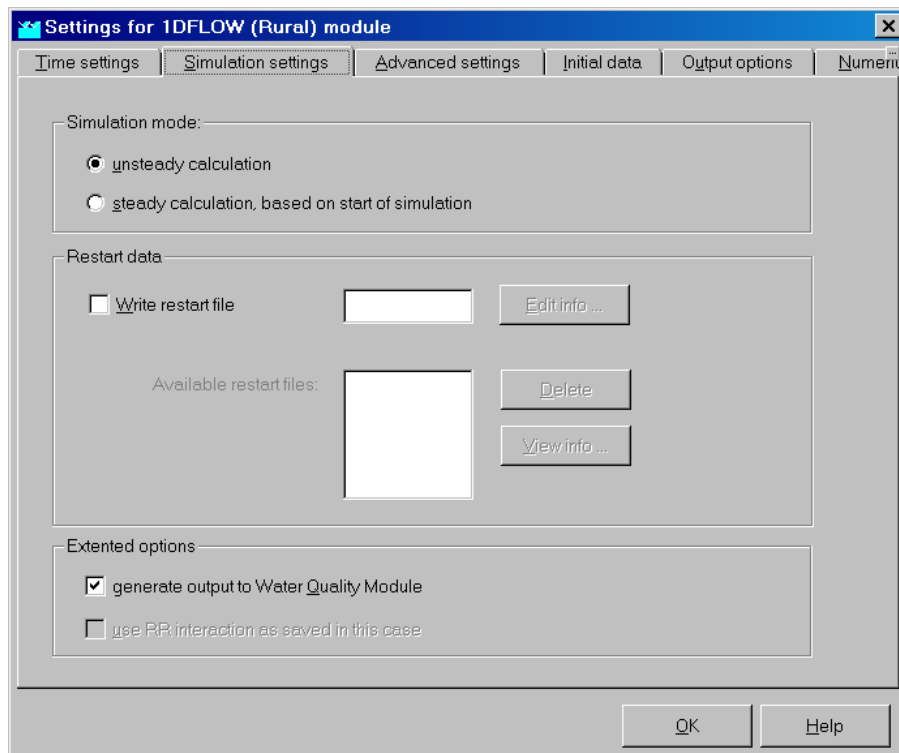
1D domain

To activate the coupling with FLOW in the 1D domain, activate the *Settings* task in the SOBEK User Interface. Select *Edit* for the “1DFLOW(Rural)” module. On the *Simulation Settings* tab form, activate “generate output to Water Quality Module” ([Figure 11.5](#)). Click *OK*.

The system may generate a warning, that the output from the 1D FLOW module will be set to mean values ([Figure 11.6](#)). This is required to run WAQ simulations.

To de-activate other coupling options with FLOW in the 3D domain, activate the *Settings* task in the SOBEK User Interface and select *Edit* for the “Delft3D-FLOW” module. On the *Time Settings* tab form:

- ◇ Select the proper <name.mdf> file at *Delft3D FLOW Master Definition Flow*.
- ◇ Select the proper <d3d_sobek_conf.ini> file in the same folder (see Manual for 1D–3D coupled hydrodynamic simulations, ([Delft3D-FLOW UM, 2013](#))).
- ◇ DO NOT activate “On-line coupling to Delft3D WAQ” ([Figure 11.7](#)).



Settings for 1DFLOW (Rural) module

Time settings | **Simulation settings** | Advanced settings | Initial data | Output options | Numerical

Simulation mode:

- ☒ unsteady calculation
- ☐ steady calculation, based on start of simulation

Restart data

☐ Write restart file [] Edit info ...

Available restart files: [] Delete View info ...

Extended options

- ☒ generate output to Water Quality Module
- ☐ use R/R interaction as saved in this case

OK Help

Figure 11.5: Settings task for “1DFLOW(Rural)” module; Simulation Settings tab form.

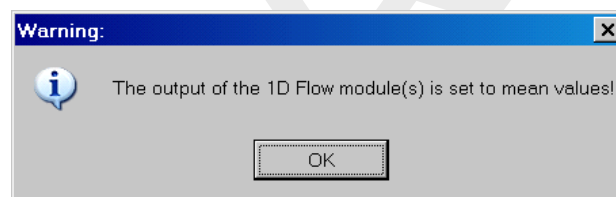
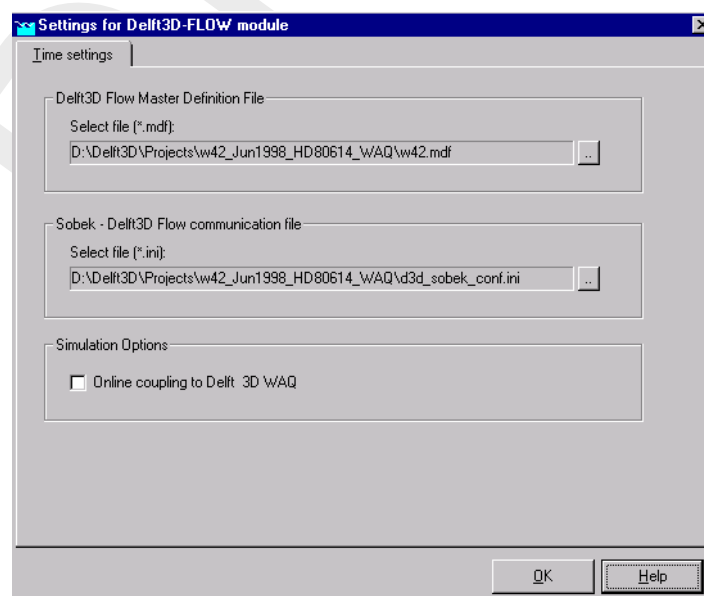


Figure 11.6: Warning message.



Settings for Delft3D-FLOW module

Time settings

Delft3D Flow Master Definition File

Select file (*.mdf):
D:\Delft3D\Projects\ww42_Jun1998_HD80614_WAQ\ww42.mdf ...

Sobek - Delft3D Flow communication file

Select file (*.ini):
D:\Delft3D\Projects\ww42_Jun1998_HD80614_WAQ\d3d_sobek_conf.ini ...

Simulation Options

- ☐ Online coupling to Delft 3D WAQ

OK Help

Figure 11.7: Settings task for “Delft3D-FLOW” module; Time Settings tab form (note that file names shown have no specific meaning).

The screenshot shows the 'Storage' tab in the FLOW-GUI interface. It contains two main sections: 'WAQ simulation times' and 'WAQ aggregation'.

WAQ simulation times

| | FLOW | WAQ |
|------------------|---------------------|---------------------|
| | dd mm yyyy hh mm ss | dd mm yyyy hh mm ss |
| Start time: | 05 08 1990 00 00 00 | 05 08 1990 00 00 00 |
| Stop time: | 06 08 1990 01 00 00 | 06 08 1990 01 00 00 |
| Time step [min]: | 5 | 5 |

WAQ aggregation

☐ Use horizontal aggregation

Select file:

Vertical aggregation

Number of FLOW layers: 10

Number of WAQ layers: 5

| | #aggr. FLW layers |
|---|-------------------|
| 1 | 1 |
| 2 | 2 |
| 3 | 2 |
| 4 | 3 |
| 5 | 2 |

<< Back

Figure 11.8: FLOW-GUI: Sub-data group Output → Storage → Export WAQ input.

3D domain

To activate the coupling with FLOW in the 3D domain, activate the Delft3D-FLOW User Interface, select *Section Output* → *Storage* → *Export WAQ input* (Delft3D-FLOW UM, 2013). Enter the desired data, for an example see Figure 11.8.



Remark:

- ◇ Note that minimum values for the vertical dispersion can not be defined at this level. Instead they can be defined in the D-WAQ user interface, see section 5.2.4.

11.5.3.2 Other input for the water quality simulation

Other input to be provided comprises for both domains:

- ◇ time frame and time step;
- ◇ selection of state variables, processes and process parameters;
- ◇ grid definition (1D domain);
- ◇ selection of numerical method;
- ◇ dispersion coefficients;
- ◇ initial concentrations;
- ◇ meteorological and other forcing functions;
- ◇ pollution loadings;
- ◇ boundary conditions (except for 1D–3D coupling boundaries);

- ◇ output definition;
- ◇ definition of observation points.

This should be done via the SOBEK (1D) and Delft3D User Interfaces. We refer to the User Manuals for further explanations ([Delft3D-FLOW UM, 2013](#); [SOBEK UM, 2013](#)).

11.5.3.3 Arranging the coupling between the 1D and 3D domains

Connecting boundaries in both domains

A coupled 1D–3D WAQ simulation presumes a successfully coupled FLOW simulation. This requires that there is correspondence between the id's of:

- ◇ the boundary nodes in the 1D domain, and
- ◇ the boundary sections in the 3D domain.

On top of that, a file named `<delft3d_sobek_waq.ini>` needs to be present in the Delft3D working directory. This file should look as follows:

```
boundaries-coupled-externally
  'name1'      175  63  177  63
  'name2'      198  75  198  75
  'name3'      216  80  216  80
...
end-boundaries-coupled-externally
```

The strings 'name1', 'name2', etc. are supposed to be equal to the names used for the coupled boundaries in the coupled 1D–3D FLOW model. The four integer numbers following the strings represent the (m, n) grid co-ordinate ranges of the corresponding boundary sections in the 3D domain. This file can be derived directly from the `<*.hyd>` file produced by the 3D FLOW simulation (if the proper arrangements are made to produce water quality files, see above).

In the D-WAQ User Interface, the boundaries will be given the name indicated in the `<delft3d_sobek_waq.ini>` file, and are indicated as — *possibly coupled* —, see [Figure 11.9](#). The boundary conditions supplied for these boundaries will be overruled by the concentrations in the corresponding branches of the 1D model during a coupled 1D–3D simulation.

Matching substances at coupled boundaries

The selection of state variables may be different in both domains. Boundary conditions however will only be exchanged at the coupling locations for state variables with the same name.

Matching time steps

The coupling is not able to deal with different time frames in both domains. Therefore, the user-defined calculation time-step must be the same in both domains, and the simulation period must be equal in both domains.

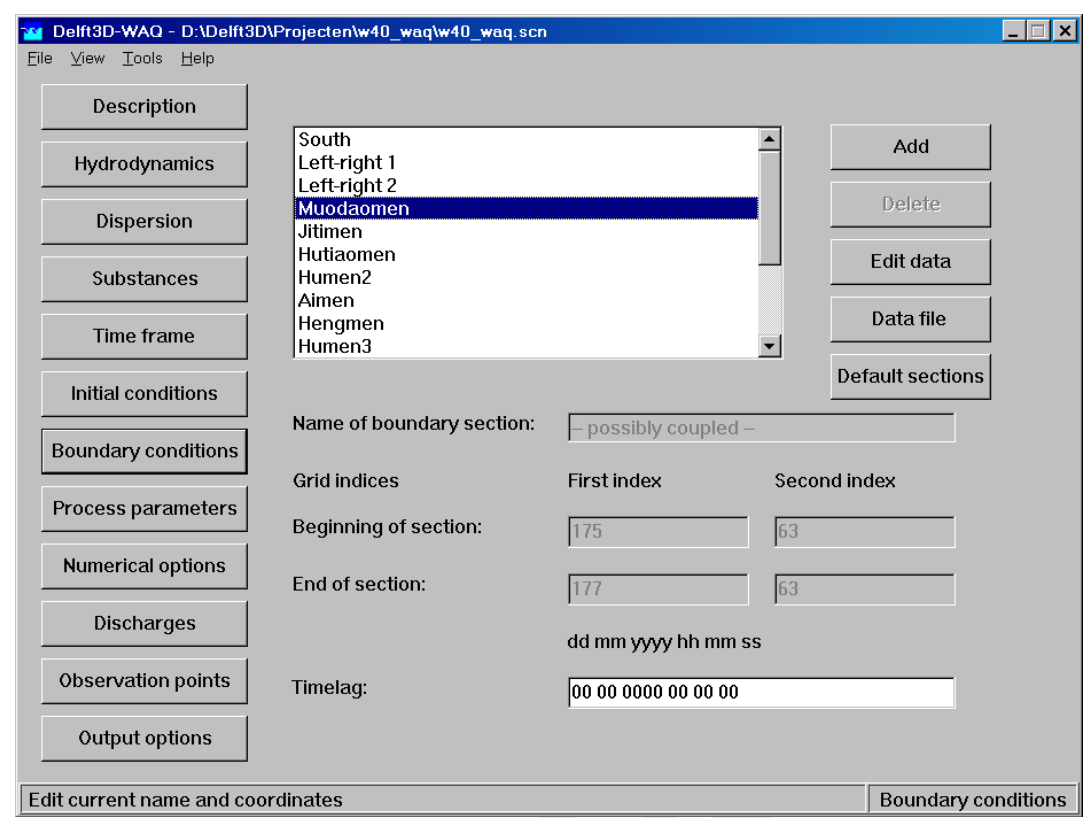


Figure 11.9: Datagroup Boundary conditions

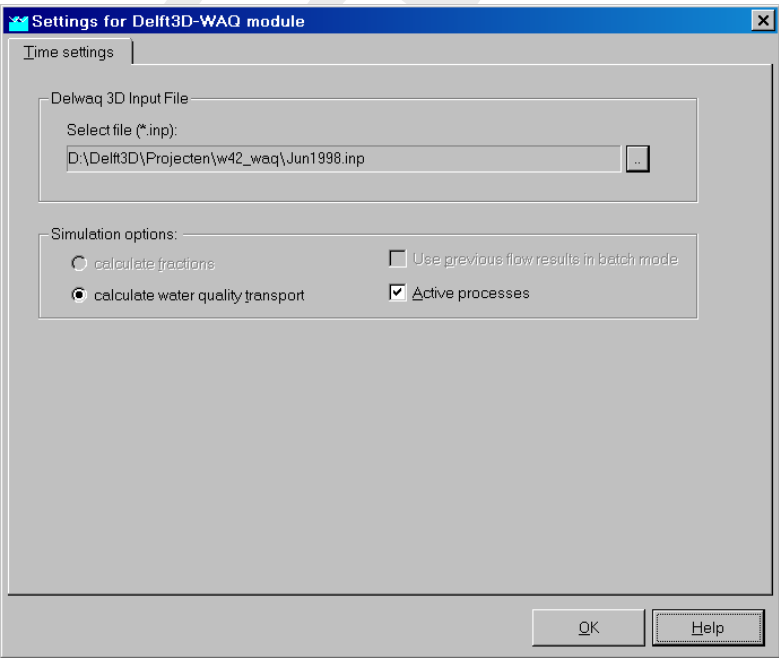


Figure 11.10: Settings for D-WAQ window (note that file name shown has no specific meaning).

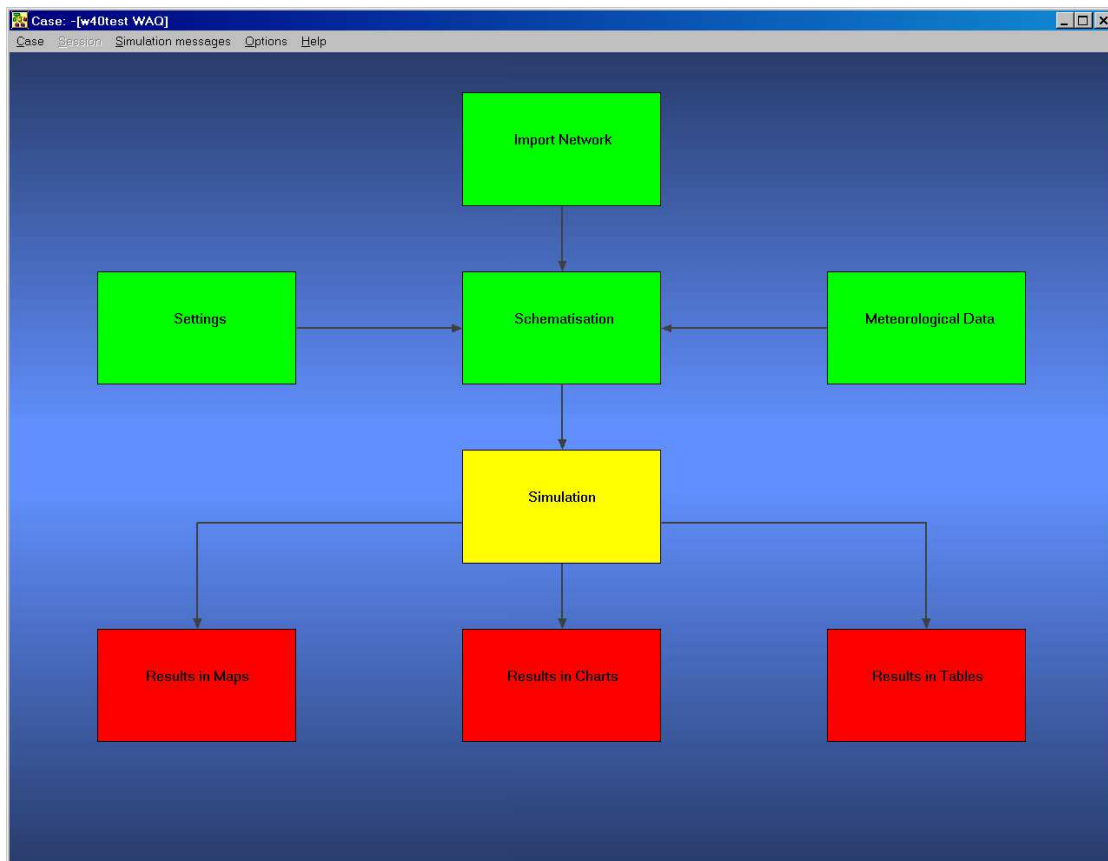



Figure 11.11: Case manager main window, ready for simulation task.

Running coupled simulations

The coupled simulation is conducted from the SOBEK User Interface. You indicate which 3D water quality input file you want to use, by activating the *Settings* task. Select *Edit* for the “D-Water Quality” module. The **Settings for Delft3D WAQ module** now appears (Figure 11.10).

On this window you define the 3D domain input file `<*.inp>`, which you prepared. This file has the same name as the `<*.scn>` file, created by the 3D domain D-WAQ GUI.

- ◇ Click on the  button next to the *Select file (*.inp)* selection box.
- ◇ Browse for and open the appropriate `<name.inp>` file.

Make sure that the rest of this window looks like Figure 11.10.

- ◇ Select *OK* to stop editing the “D-Water Quality” module.
- ◇ Select *OK* to leave the Settings task box.

To run a simulation, double-click the *Simulation* task box (see Figure 11.11).

You will be prompted to use the water quantity (FLOW) results from a previous simulation (Figure 11.12). Click *Yes*.

You will be warned that existing output for the 3D water quality domain will be overwritten. Verify that this is not a problem, and click *Yes* (Figure 11.13).

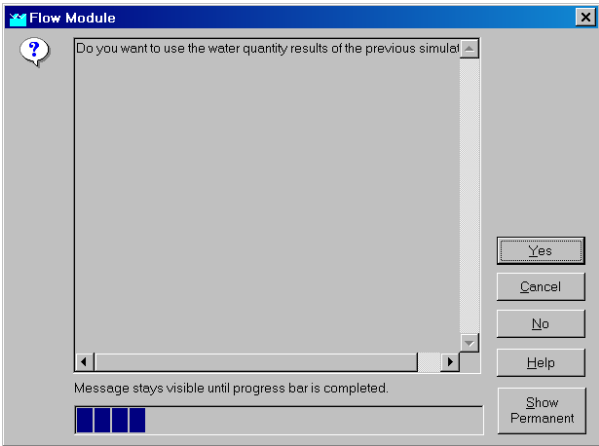


Figure 11.12: Simulation task Flow Module window.

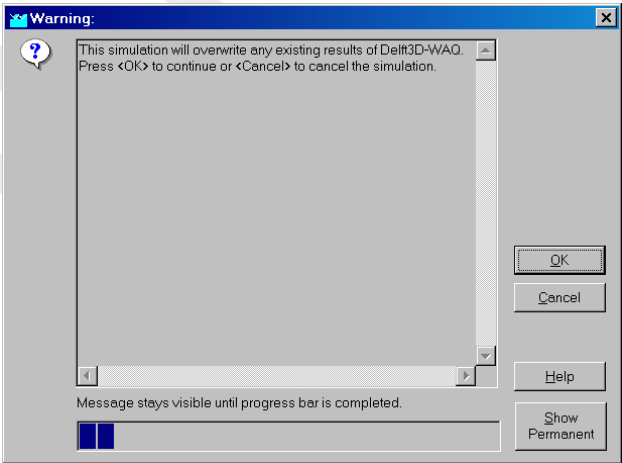


Figure 11.13: Simulation task; warning for overwriting D-WAQ results.

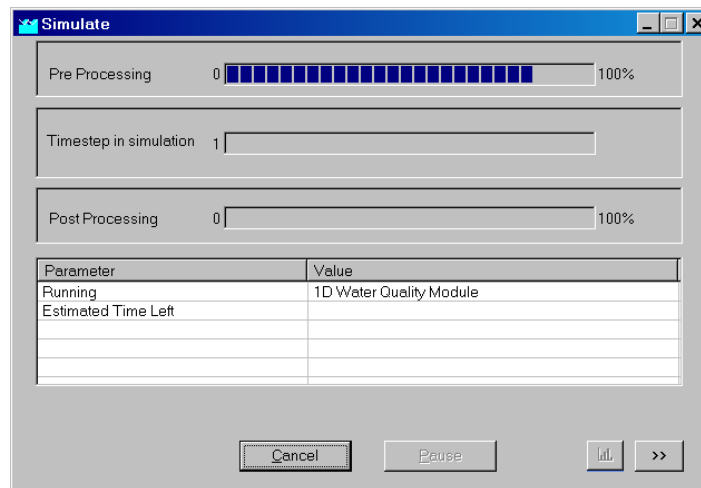


Figure 11.14: Simulation task progress window; pre-processing.

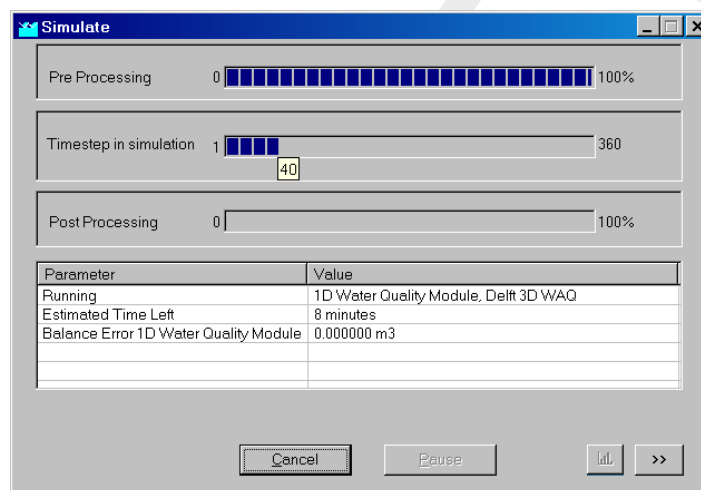


Figure 11.15: Simulation task progress window; processing.

The simulation task will proceed with pre-processing tasks (Figure 11.14), simulations (Figure 11.15) and post-processing tasks.

When the simulation is successfully completed, the main window will be like Figure 11.16.

If problems are encountered, move the mouse to the *Simulation* task box, and use the right mouse button to access report files:



Figure 11.17: Accessing Help and Simulation messages

The relevant messages files are:

- ◇ 1D domain
 - input reports: <delwaq.lst> and <delwaq.lsp>
 - simulation report: <delwaq.mon>

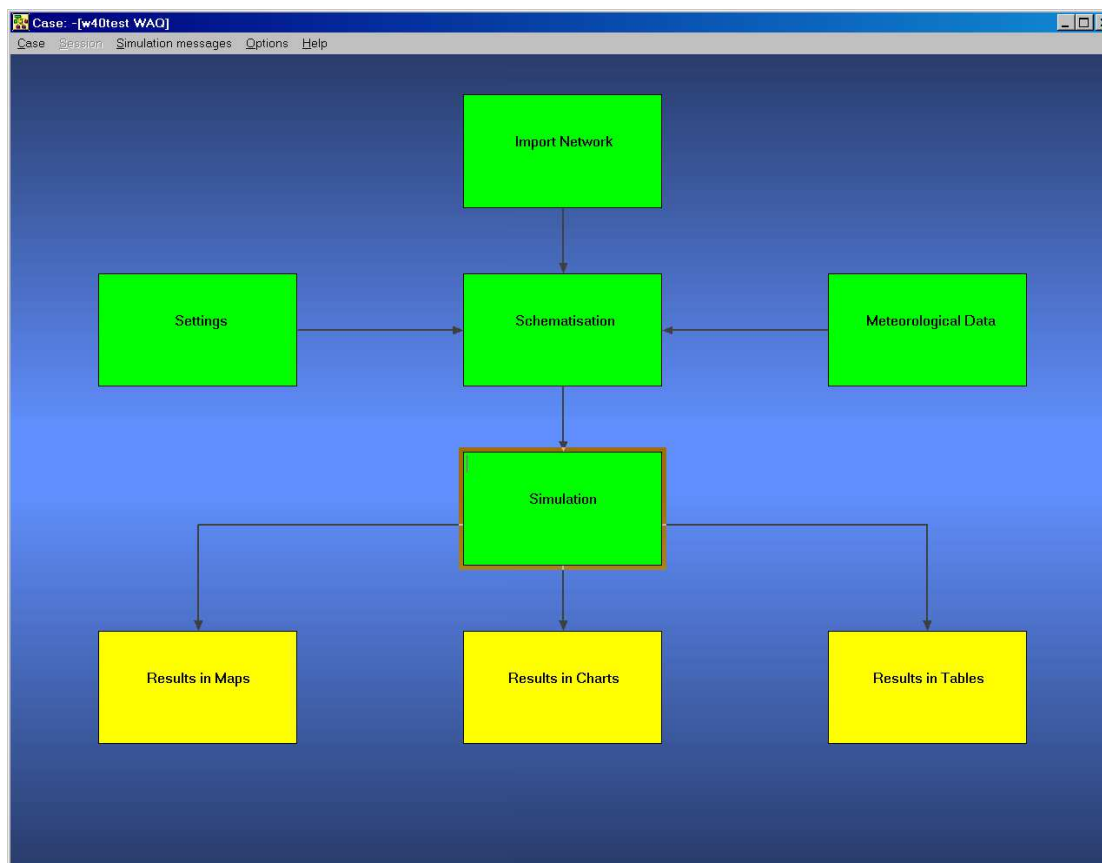


Figure 11.16: Case manager main window, simulation task successfully completed.

◇ 3D domain

- input report: `<name.lst>` and `<name.lsp>`
- simulation report: `<name.mon>` where *name* is the name of the *.inp used.

11.5.4 Tips & Tricks

The `<*.mon>` simulation report file from both domains provides feed back on the successful matching of boundaries and state variables. In the top section of both files you should find lines looking like:

```

Domain decomposition boundary matching for:delwaq_to_xxxx
for boundary 1 (South)          no match found
...
for boundary 309 (West)         no match found
for boundary nMuodaomen         match found with number:    3324
for boundary nMuodaomen         match found with number:    3324
for boundary nMuodaomen         match found with number:    3324
...
...

Domain decomposition substance matching for:delwaq_to_xxxx
for substance AAP               match found with number:    1
for substance DetC              match found with number:    2
...
for substance CbodU             no match found
...
  
```

Evidently, it is possible that some boundaries and substances show no match. You have to

take care however, that all boundaries and substances which are supposed to match between both domains, are actually matching.

DRAFT

DRAFT

References

List of related publications

General:

- ◇ Baptist and De Vries (1998)
- ◇ Bent *et al.* (1991)
- ◇ Jenkins *et al.* (1997)
- ◇ Salden *et al.* (1996)
- ◇ Vatvani and Montazeri (1989)
- ◇ Vos (1995a)
- ◇ Vos and Schuttelaar (1995b)
- ◇ Vos *et al.* (1998a)
- ◇ Vos *et al.* (1998b)
- ◇ WL | Delft Hydraulics (1994a)
- ◇ WL | Delft Hydraulics (1996a)
- ◇ WL | Delft Hydraulics (1997b)
- ◇ WL | Delft Hydraulics (1999)

Sediment:

- ◇ Flokstra and Jagers (1999)
- ◇ Kranenburg and Winterwerp (1997a)
- ◇ Kranenburg and Winterwerp (1997b)
- ◇ Mosselman *et al.* (1999)
- ◇ ?
- ◇ Vos and Gerritsen (1997)
- ◇ Vos *et al.* (1998b)
- ◇ Winterwerp (1999a)
- ◇ Winterwerp (1999b)
- ◇ Winterwerp *et al.* (1998)
- ◇ WL | Delft Hydraulics (1996b)
- ◇ WL | Delft Hydraulics (1997a)
- ◇ WL | Delft Hydraulics (2000)

Ecology:

- ◇ Los and Bokhorst (1997)
- ◇ Van der Molen *et al.* (1994)
- ◇ Peeters *et al.* (1995)
- ◇ De Vries *et al.* (1998)
- ◇ WL | Delft Hydraulics (1991a)
- ◇ WL | Delft Hydraulics (1994b)
- ◇ WL | Delft Hydraulics (1996b)
- ◇ WL | Delft Hydraulics (1997c)
- ◇ WL | Delft Hydraulics (1997d)
- ◇ WL | Delft Hydraulics (1998a)
- ◇ WL | Delft Hydraulics (1998b)



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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] | Couple | WAQ(2) |
| *.atr | Model schematisation file containing the attributes of the computational cells. Attributes indicate the vertical position of the computational cell: 0 = 2D simulation 1 = surface layer 2 = intermediate layer 3 = bottom layer | Couple | WAQ(2) |
| *-bal.his | Result file with mass balances per observation point for each substance | WAQ(2) | GPP |
| *.cco | Model schematisation file containing the coordinates of the computational grid. Always accompanied by <*.lga> file | Couple | WAQ-GUI GPP |
| *.chz | Model schematisation file containing Chézy values of the computational cells | Couple | – ¹ |
| *.did | Configuration file for the horizontal aggregation tool DIDO | DIDO | DIDO |
| *.dmo | File with name and segment numbers of monitoring areas in ASCII format. | DIDO | WAQ-GUI |
| *.dsp | ASCII file with dispersion array that overrules the uniform dispersions specified | – | WAQ-GUI WAQ (1) |
| *.dwq | Horizontal aggregation file | DIDO | Couple |
| continued on next page | | | |

Table A.1 – continued from previous page

| File extension | Description | Output from | Input for |
|------------------------|---|-------------|----------------|
| *.flo | Model schematisation file containing the flows between computational cells in [m ³ /s] | Couple | 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 |
| *.his | Result file with time-series information at observation points in binary format | WAQ(2) | GPP |
| *.hyd | Coupled hydrodynamics information file | Couple | WAQ-GUI |
| *.ini | Initial condition for the water quality simulation. (File size only greater than zero when spatially varying initial conditions are used.) | WAQ-GUI | WAQ(1) |
| *.inp | Input file for water quality simulation | WAQ-GUI | WAQ(2) |
| *.len | Model schematisation file containing the dispersion lengths of computational cells in [m] | Couple | WAQ(2) |
| *.lga | Model schematisation file containing numbering of computational cells | Couple | WAQ-GUI GPP |
| *.lgo | (not used) | – | – |
| *.lgt | (not used) | – | – |
| *.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) | WAQ-GUI GPP |
| *-stat.map | Result file with spatial information of statistical output | WAQ(2) | GPP |
| continued on next page | | | |

Table A.1 – continued from previous page

| File extension | Description | Output from | Input for |
|------------------------|---|-------------------|----------------|
| *.mhy | Multiple hydrodynamics file to describe a water quality simulation that makes use of more than one hydrodynamic <*.hyd> files | WAQ-GUI | WAQ-GUI |
| *.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) | – |
| *.obs | File with name and location (x, y, z) of observation points in ASCII format | – | WAQ-GUI |
| *.par | Parameter file containing process parameters that are spatially varying, but constant in time | WAQ-GUI | WAQ(1) |
| *.poi | Model schematisation file containing the linkages (pointers) between the computational cells | Couple | WAQ(2) |
| *.q3d | QUICKIN 3D data file | QUICKIN | WAQ-GUI |
| *.qin | QUICKIN data file | QUICKIN | WAQ-GUI |
| *.res | 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 | Couple | – ¹ |
| *.scn | Scenario file describing the set-up of a water quality simulation | WAQ-GUI | WAQ-GUI |
| *.src | Flow rates in [m ³ /s] for each discharge derived from the hydrodynamic simulation | Couple | WAQ-GUI |
| *.srf | Model schematisation file containing the horizontal surface areas of the computational cells in [m ²] | Couple | WAQ-GUI |
| *.stt | Input file for specifying statistical output for a water quality simulation | WAQ-GUI 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 | WAQ-GUI |
| continued on next page | | | |

Table A.1 – continued from previous page

| File extension | Description | Output from | Input for |
|------------------------|---|--------------|----------------|
| *.tau | Shear stress values (Tau) in [N/m ²] derived from the hydrodynamic simulation through the <com-*.dat> file | Couple | – ¹ |
| *.tem | Water temperature values in [°C] derived from the hydrodynamic simulation through the <com-*.dat> file | Couple | – ¹ |
| *.tim | Time-series file to import process parameters, boundary conditions or discharges into the WAQ-GUI | – | WAQ-GUI |
| *.vol | Model schematisation file containing the volumes of the computational cells in [m ³] | Couple | 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 | Couple | 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. | Couple | WAQ(2) |
| breakp.dat | (not used) | – | – |
| com-*.dat | Communication file. Result file from the hydrodynamic (Delft3D-FLOW) simulation in NEFIS format containing all relevant information such as model schematisation, flow rates, etc. Always accompanied by the <com-*.def> file | Delft3D-FLOW | Couple GPP |
| com-*.def | NEFIS definition file of <com-*.dat> file | Delft3D-FLOW | Couple GPP |
| couplnef.out | Report file of the coupling containing information on model schematisation and aggregation, minimal residence times and closure errors | Couple | – |
| d3d_waq.log | Log file that keeps track of the actions carried out with the WA- GUI in the current working directory | WAQ-GUI | – |
| d3d_menu.msg | Contains messages from the Delft3D-MENU | Delft3D-MENU | – |
| continued on next page | | | |

Table A.1 – continued from previous page

| File extension | Description | Output from | Input for |
|----------------|--|-------------|-----------|
| del*.inp | Basic input file for a water quality simulation using the substance Continuity; based on the information in the <com-*.dat> file | Couple | – |
| delw420.dat | Framework for the basic input file <del*.inp>. Information derived from the <com-*.dat> file is filled in | – | Couple |
| delwaq.rtn | (not used) | – | – |
| matrix.dat | (not used) | – | – |
| pointer.asc | Model schematisation file containing the linkages (pointers) between the computational cells. ASCII version of the <*.poi> file | Couple | – |
| substate.rtn | (not used) | – | – |
| waq_gui.err | Error messages from the WAQ-GUI | – | – |

¹ Optionally, these files can be used as segment functions for their respective equivalents in the WAQ-GUI

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-WAQ and need not be defined here. You will never have to deal with their formats.

Some files are described elsewhere in the D-WAQ User Manual:

- 1 <*.lst> Refer to [section 6.1.2](#).
- 2 <*.lsp> Refer to [section 6.1.3](#).
- 3 <*.mon> Refer to [section 6.2.1](#).

A.2.1 Observation file <*.obs>

The observation file <*.obs> can be used to import observation points in the WAQ-GUI. Information you need to specify are the name (max 20 characters) of the observation point, its horizontal position in the co-ordinate system that is used to define the model grid and a layer number for its vertical position. The file format is prescribed, the order of the columns can not be changed:

```
# Structure of an <*.obs> file:
# The file is a comma-separated ASCII-file,
#           containing a header and on each line an observation point.
# The format of the header is fixed!
# The header contains: x-co-ordinate, y-co-ordinate, layer, name
# If layer is 0 then it will be "Uniform over depth".
#
#
# Example:
#
```

```
#   x,      y, layer, name
18000, 22625,     1, central obs-point
13373, 11621,     0, south-western obs-point
22462, 23552,     4, north-western obs-point
```

A.2.2 Observation area file <*.dmo>

Observation areas are collections of individual computational cells, the concentration in each cell is averaged and the mass balances, if any, are computed for the cells as a whole. There can be only one such file and the contents can not be edited. Instead you can use a program like D-Waq DIDO to generate the file.

Files with observation areas are supposed to have the following layout:

```
# structure of a <*.dmo> file:
# The file may contain comment lines at the start
# After the comments:
# - The number of observation areas
# - Per observation area:
#   - the name (enclosed in single quotes, max 20 characters)
#   - the number of grid cells in the observation areas
#   - a list of indices of grid cells (separated by spaces)
#
# Example:
2
'Area_1' 5
1 2 3 4 5
'Area_2' 4
6 7 8 9
```



Remark:

- ◇ Between the last comment line and the line with the number of areas, there may not be a blank line.

A.2.3 Time-series file <*.tim>

The general time-series file as supported by the Delft3D system is an ASCII text file containing keywords and values that are separated by any number of spaces, tabs or commas¹. We distinguish the following keywords:

table-name '<table>'²

The keyword indicates the beginning of a new table. It is obligatory if there is more than one table in the file. If it is missing, the reading program will assume that there is only one single table. This table will get the name of the file.

Note that names are placed in single quotes ('), so as to allow spaces, tabs and commas. They can be at most 40 characters long.

contents '<contents>'

The *contents* keyword must follow the table name. The string that is filled in here has meaning to the interpretation of the table. Within Delft3D only the FLOW module currently uses this keyword to specify the vertical distribution of the boundary values. The following options are used:

1 *uniform*

This indicates a vertically uniform boundary condition. The values must be given at

¹Important: double tabs or double commas are not assumed to indicate a missing value. Missing values need to be identified by the special value -999.0.

²Fields that can be filled at liberty are enclosed in triangular brackets (<>). Optional fields are enclosed in square brackets ([]).

both ends of the boundary section.

2 *linear*

A linear profile for the vertical distribution is assumed. Values must be given at the surface layer for the beginning of the section (end A), for the bottom layer at end A, for the surface layer at end B and for the bottom layer at end B.

3 *step*

Besides the values at the surface and bottom at both ends (like linear) also the depth of the discontinuity must be given.

4 *3d-profile*

Values must be given at all layers and for both ends. This options is especially useful when using in conjunction with a model for a larger area (nesting).

location '*<location>*'

The name of the location has no consequences for the interpretation of the table's contents and serves as documentation or identification.

geo-coordinates *<long>* *<lat>* [*depth*]

Specifies the geographical co-ordinates of the point in question (in degrees longitude and latitude). The depth is optional (in metres relative to a reference level). This keyword is also mainly for documentation and identification.

metric coordinates *<x>* *<y>* [*depth*]

Specifies the metric co-ordinates of the point in question (in metres). The depth is optional (in metres relative to a reference level). An alternative is:

metric coordinates *<x>* *<y>* *layer* *<layer number>*

To accommodate for the situation that the model layer has to be specified. Note that the layer indication should be a negative number counting from the top (being -1 and then -2 ... till the bottom -number_of_layers).

time-function '*astronomic*' '*harmonic*' '*equidistant*' '*non-equidistant*'

This keyword indicates how to interpret the numbers:

1 *astronomic*

The table contains astronomical tidal components, with the first column containing the names of these components. For each parameter the amplitude and the phase are to be given next to each other. The phase is always expressed in degrees.

2 *harmonic*

The table contains harmonic components, with in the first column the angular velocity or the period of the components. For each parameter both amplitude and phase are to be given next to each other.

3 *equidistant*

The table contains a time-series with equidistant times. The keyword to specify the time step must be present. The first column contains the value of the first parameter, because the time is implicit.

4 *non-equidistant*

The table contains a time-series with arbitrary times. The first column specifies the time, because in this case the time must be given explicitly. The second column contains the value of the first (real) parameter, and so on. This is the default.

constant

To enter a constant function it is enough to specify this keyword: a single set of values is expected, one for all parameters.

reference-time *<yyyymmdd>* *<hhmmss>* [*<yyyymmdd>* / *from model*]

The time can be specified relatively or absolutely. Sometimes it is convenient to define a start time and the subsequent times in hours or minutes from that start time. This start time or reference time can be taken from the model that will use the data or be specified in the form year-month-day, hour-minute-seconds.

time-unit 'date' /'years' /'decades' /'days' /'hours' /'minutes' /'seconds' /'ddhhmmss'

The unit in which the relative time is expressed can vary widely, hence the various units. If the time is given absolutely, then this is recognised via the keyword *date* (date and time in the form *yyyymmdd hhmmss*). Should the keyword be absent and no reference time be given, then the first time is used to identify whether an absolute or a relative time is used.

time-step <value>

The time step needs to be given only for equidistant time-series. The value must be expressed in the correct unit (if unit of time is *date*, then the time step must be expressed as *dddhhmmss* - months have little importance then).

interpolation 'linear' /'block'

With this keyword the method of interpolation is indicated. It only has meaning for time-series. *Linear* means: linear interpolation between the given times, *block* means that the value of the last time holds up to the next time.

extrapolation 'periodic' /'constant' /'none'

With this keyword the method of extrapolation is indicated: How to determine the value for times that fall outside the interval of the time-series? It only has consequence for time-series (not for harmonic or astronomic series). *Periodic* means: the time-series is assumed to be periodic. In the case *constant* the value outside the interval is set equal to that at the nearest time. The method *none* causes an error, when the time is outside of the interval.

parameter '<parameter>' unit '<unit>'

This keyword is used both to identify the column and to specify the number of columns: one such line must appear for each column in the table. This way you are free to specify the numbers on one or more lines, just as it suits your purposes. Be careful not to add too many or too few numbers per time, as the reading program may not be able to detect this.

records-in-table <number>

This keyword is mainly used within the Delft3D-FLOW set-up to make reading the file more simple. It indicates the number of records. If used, it should be placed right before the actual data.

comments (any text after an asterisk or a hash)

Text that appears after an asterisk (*) is ignored as well as that after a hash (#). This allows you to add documentary texts.

Most keywords can appear in any order, except for *contents* and *parameter*, as these have a specific meaning. The skeleton of the table does look like this:

```
table-name 'table'
  contents 'contents'
  .... keywords representing options
  parameter ...
  parameter ...
  ...
  [records-in-table <number>]
  <time> <value1> <value2> ...
  <time> <value1> <value2> ...
  ...

table-name ..
...
```

Examples:

```
# Time-series file for input parameter
table-name 'Windspeed\_1998'
# Wind data derived from station East
contents 'wind speed 1998'
```

```

time-unit      'days'
reference-time  19980101 000000
time-function  'non-equidistant'
parameter      'time' unit 'days'
parameter      'Wind speed' unit 'm/s'
parameter      'Direction' unit 'degrees'
0      3      110
0.125   2      80
0.25    1      70
0.375   2     130
0.5     5     120
0.625   6     130
0.75    4     110
0.875   3     110
1      3     110

* Time-series file for multiple discharges
table-name 'River Shiny'
contents 'waste load data'
  location 'River Shiny'
  metric coordinates 291477 1608157 layer 0
  time-unit 'days'
  reference-time 19960101 000000
  time-function 'non-equidistant'
  parameter 'time' unit 'days'
  parameter 'Salinity' unit '[-]'
  parameter 'IM1' unit '[-]'
  parameter 'TColi' unit '[-]'
  parameter 'NH4' unit '[-]'
  parameter 'NO3' unit '[-]'
  parameter 'PO4' unit '[-]'
  parameter 'DetC' unit '[-]'
* time Sal. IM1 TColi NH4 NO3 PO4 DetC
0 0.997E+03 0.5781E+03 0.5548E+01 0.6410E+01 0.5707E+02 0.1130E+02 0.5890E+02
1 0.976E+03 0.5660E+03 0.5432E+01 0.6276E+01 0.5588E+02 0.1107E+02 0.5767E+02
2 0.956E+03 0.5542E+03 0.5319E+01 0.6145E+01 0.5471E+02 0.1084E+02 0.5647E+02
3 0.936E+03 0.5427E+03 0.5208E+01 0.6018E+01 0.5358E+02 0.1061E+02 0.5530E+02
4 0.917E+03 0.5315E+03 0.5101E+01 0.5894E+01 0.5247E+02 0.1039E+02 0.5415E+02
5 0.898E+03 0.5206E+03 0.4996E+01 0.5773E+01 0.5140E+02 0.1018E+02 0.5304E+02
table-name 'Discharge Dwarf'
contents 'waste load data'
  location 'River Dwarf'
  metric coordinates 295041 1612697 layer 0
  time-unit 'days'
  reference-time 19960101 000000
  time-function 'non-equidistant'
  parameter 'time' unit 'days'
  parameter 'Salinity' unit '[-]'
  parameter 'IM1' unit '[-]'
  parameter 'TColi' unit '[-]'
  parameter 'NH4' unit '[-]'
  parameter 'NO3' unit '[-]'
  parameter 'PO4' unit '[-]'
  parameter 'DetC' unit '[-]'
* time Sal. IM1 TColi NH4 NO3 PO4 DetC
0 0.596E+02 0.6017E+01 0.3352E+00 0.1120E+01 0.2635E+01 0.6340E+00 0.3036E+01
1 0.581E+02 0.5870E+01 0.3270E+00 0.1092E+01 0.2570E+01 0.6185E+00 0.2961E+01
2 0.570E+02 0.5759E+01 0.3208E+00 0.1072E+01 0.2522E+01 0.6068E+00 0.2905E+01
3 0.556E+02 0.5611E+01 0.3126E+00 0.1044E+01 0.2457E+01 0.5912E+00 0.2831E+01
4 0.545E+02 0.5501E+01 0.3064E+00 0.1023E+01 0.2409E+01 0.5796E+00 0.2775E+01
5 0.537E+02 0.5427E+01 0.3023E+00 0.1010E+01 0.2376E+01 0.5718E+00 0.2738E+01

```

A.2.4 Dispersion array <*.dsp>

The dispersion array can be used to apply spatially non-uniform dispersions. A dispersion is defined for each exchange between computational cells. Within D-WAQ each exchange has a unique number that identifies it.

If you want to apply non-uniform values you first have to indicate the default value and then you have to specify for which exchanges you want to use a different value. The major question is to know the exchange numbers. Follow this procedure:

- 1 Identify the segment numbers of the computational cells in between which the exchange is located. You can use GPP for this purpose.
- 2 Then use the <pointer.asc> file of the hydrodynamic simulation you are using, to find the exchange number.

For example, we want to use the exchange number between computational cells 111 and 112. The line in the <pointer.asc> file might look like this:

```

NO.   FROM  TO   FROM-1 TO+1      FROM-LEN  TO-LEN
....
111   111   112   110    113      773.186    760.346

```

The first column is the exchange number we're after. The second to fifth column are segment numbers. For the dispersion array you are only interested in the second and third column, ignore the fourth and further columns. So we see that exchange number '111' links the computational cells '111' and '112'.

The dispersion array file <*.dsp> then looks like this:

```

2                ; 2 = option "additional dispersion with default"
1.0  5.0         ; scale factor and default dispersion in the first direction
3                ; number of overridings in the first direction
exchange_#1      new_dispersion_value
exchange_#2      new_dispersion_value
exchange_#3      new_dispersion_value
1.0  5.0         ; scale factor and default dispersion in the second direction
2                ; number of overridings in the second direction
exchange_#4      new_dispersion_value
exchange_#5      new_dispersion_value
1.0  1.e-6       ; scale factor and default dispersion in the third direction
0                ; number of overridings in the third direction

```



Note: that you have to specify the dispersion in three directions in case of a 3D simulation, in two direction in case of a 2DH or 2DV simulation and in one direction in case of a 1D simulation. Further note that the third direction by definition is the vertical direction.

A.2.5 Simple locations/table <*.*)>

The Simple locations/table file has no prescribed file extension. The file type can be used to import time-series for process parameters, boundaries or discharges. The comma-separated file looks like this:

```

Location, X, Y, Z, Time,      "Salinity", "NH4", "Sups.solids", "RcNit"
                                "g/l", "mg/l", "mg/l", "l/d"
                                1.0,1.0,1.0,1.0
"Location 1", 15000., 20000., 0., 2000/01/01-00:00:00, 30.0, 1.0, 100.0,0.1

```

```

                                2000/02/01-00:01:00, 31.0, 1.1, 120.0,0.15
                                2000/03/04-12:53:00, 28.0, 3.1, 120.0,0.12
"Location 2", 15000., 15000., 1., 2000/01/01-00:00:00, 30.4, 1.0, 100.0,0.25
                                2000/02/01-00:00:00, 31.4, 1.1, 120.0,0.3

```

The first three lines and the first 5 columns are fixed:

1 Lines

- 1.1 line 1: header with column names, sixth column and further must be between double quotes ""!
- 1.2 line 2: units, only for the sixth column and further, must be between double quotes ""
- 1.3 line 3: scale factors, only for the sixth column and further, must be real values (no integers)

2 Columns

- 2.1 column 1: Name of locations, must be between double quotes ""
- 2.2 column 2: x co-ordinate, must be real value (no integer)
- 2.3 column 3: y co-ordinate, must be real value (no integer)
- 2.4 column 4: layer number, must be real value (no integer)
- 2.5 column 5: absolute timers, format yyyy/mm/dd-hh:mm:ss

If a location has more than one timer, the first to fifth column must be left blank.

A.2.6 Segment function <*.*>

A segment function has 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).

For Fortran the program can look like this:

```

      PROGRAM WRITE_SEGENT_FUNCTION
      PARAMETER (NOSEG=10, NOTIME=5)
C
C NOSEG = Number of segments
C NOTIME = Number of time steps
C
      REAL      VALUE(NOSEG, NOTIME)
      INTEGER   TIMER
C
      DO 10 I=1, NOTIME
        DO 11 J=1, NOSEG
          VALUE(I,J)= ???  !! some kind of formula, fill the matrix
11      CONTINUE
10     CONTINUE
C
      OPEN (15, FILE='segmentfunction.bin',FORM='BINARY')
C
      DO 20 I=1, NOTIME
        TIMER = (I-1) * 86400
        WRITE (15_) TIMER, (VALUE(I,J), I=1, NOSEG)
20     CONTINUE
      CLOSE (15_)
      END

```

Each record contains one time step consisting of a timer (**in seconds**) and as many parameter values as there are segments (NOSEG). The number of segment can be found in the input file <*.inp>, search for 'number of segments' in the <*.inp> file.

The timer is relative from the reference time in your simulation. So if the reference time is for example February 1, 2003, then on February 15, 2003 00:00 the timer equals 1209600 seconds. In the example above a time step of one day (86400 seconds) is applied.

A.2.7 QUICKIN data file <*.qin>

This file applies to 2D models.

Initial conditions for substances or space varying process parameters can be specified using a QUICKIN file per substance or parameter.

See the FLOW User Manual for a detailed description of the format of this file.

| | |
|---------------|---|
| File contents | The bathymetry in the model area, represented by depth values (in metres) for all grid points. |
| Filetype | ASCII |
| File format | Free formatted or unformatted |
| Filename | <name.dep> |
| Generated | FLOW-GUI (only for uniform depth values). Offline with QUICKIN and data from digitised charts or GIS-database. |

Record description:

| Filetype | Record description |
|----------------|--|
| Free formatted | Depth values per row, starting at N = 1 to N = Nmax, separated by one or more blanks. The number of continuation lines is determined by the number of grid points per row (Mmax) and the maximum record size of 132. |
| Unformatted | Mmax depth values per row for N = 1 to N = Nmax. |



Restrictions:

- ◇ The file contains one M and N line more than the grid dimension.
- ◇ The maximum record length in the free formatted file is 132.
- ◇ Depth values from the file will not be checked against their domain.
- ◇ The input items are separated by one or more blanks (free formatted file only).
- ◇ The default missing value is: -999.0

Example:

File containing 16 * 8 data values for a model area with 15 * 7 grid points (free formatted file).

```

1.0    2.0    3.0    4.0   -5.0   -5.0   -5.0    8.0    9.0   10.0   11.0
12.0   13.0   14.0   -5.0 -999.0
3.0    4.0    5.0    6.0    7.0   -6.0   -6.0   10.0   11.0   12.0   13.0
14.0   15.0   16.0   17.0 -999.0
5.0    6.0    7.0    8.0    9.0   10.0   -7.0   12.0   13.0   14.0   15.0
16.0   17.0   18.0   19.0 -999.0
7.0    8.0    9.0   10.0   11.0   12.0   13.0   14.0   15.0   16.0   17.0

```



```

18.0  19.0  -7.0  19.0 -999.0
 9.0  10.0  11.0  12.0  13.0  14.0  15.0  16.0  17.0  18.0  19.0
20.0  19.0  18.0  17.0 -999.0
-7.0  12.0  13.0  14.0  15.0  16.0  17.0  18.0  19.0  20.0  19.0
18.0  17.0  16.0  15.0 -999.0
-8.0  -8.0  15.0  16.0  17.0  18.0  19.0  20.0  19.0  18.0  17.0
16.0  15.0  14.0  13.0 -999.0
-999.0 -999.0 -999.0 -999.0 -999.0 -999.0 -999.0 -999.0 -999.0 -999.0
-999.0 -999.0 -999.0 -999.0 -999.0

```

Remarks:

- ◇ Each substance or parameter requires a separate QUICKIN file.
- ◇ The file generated by QUICKIN is the so-called depth file. If necessary rename the <*.dep> file to <*.qin>.
- ◇ If you have aggregated the grid then you prepare the QUICKIN data file using the (original) un-aggregated grid. The substance value for the aggregated grid cell is then taken from the first un-aggregated cell in the aggregated cell.

**Warning:**

- ◇ For substances specified in gram/cell you can not use the QUICKIN data files if the grid is aggregated.

**A.2.8 QUICKIN 3D data file <*.q3d>**

This file applies to 3D models.

The format of the 3D QUICKIN file to be used as initial condition (or process parameter) for a 3D WAQ model is:

- ◇ For each layer you have to specify the initial condition in a block. The format of the block is exactly the format of the QUICKIN depth file.
- ◇ First layer 1 (surface) then layer 2, etc.

Remark:

- ◇ The file applies to only 1 substance.



So, first you make the 'depth' file for layer 1, save it in QUICKIN as subs_lay_1.dep; next for layer 2, save it as subs_lay_2.dep.; etc.

Then you copy subs_lay_1.dep to subs_1.q3d. Open it and copy the contents of subs_lay_2.dep AT THE END. Then open subs_lay_3.dep and COPY this one at the end. etc. Finally save the file subs_1.q3d.

DRAFT

B Standard substance files

B.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.

B.2 Salinity and tracers (fractions)

B.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> |



B.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 $1/(2*30) = 0.017/\text{day}$. That is: 0.005/day would do as well as 0.05/day, but not 1/day.

B.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:

$$\frac{[dTrace_i]}{dt} = -k_{decay}[dTrace_i] \quad (\text{B.1})$$

To determine the "age" T of the water as it has come from the source:

$$T_i = -\frac{1}{k_{decay}} \ln([dTrace_i]/[cTrace_i]) \quad (\text{B.2})$$

| 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 | — |

| Input item | Description | Unit | Default value | Editable | Range |
|------------|---------------------------------|------|-------------------|----------|-------|
| T_i | "age" (travel time) of tracer i | d | output of process | – | – |

B.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.

B.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 |

B.3 Basic coliform model

B.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:

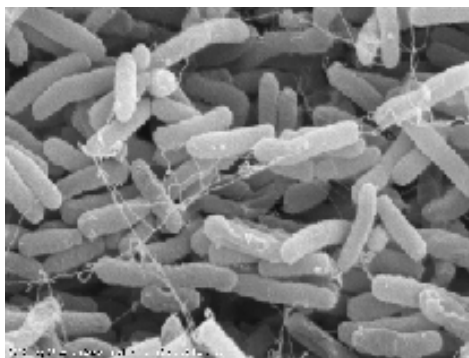
| | |
|-------------------------|---------------|
| Name of PLCT input file | <coli_04.0> |
| Name of substance file | <coli_04.sub> |

B.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 | | | |

B.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.

$$Flux = ((Rc_0 + Mrt_{Cl}) \times \vartheta^{T-20} + Mrt_{Rad}) \times [E.Coli] = Mrt_{E.Coli} \times [E.Coli]$$

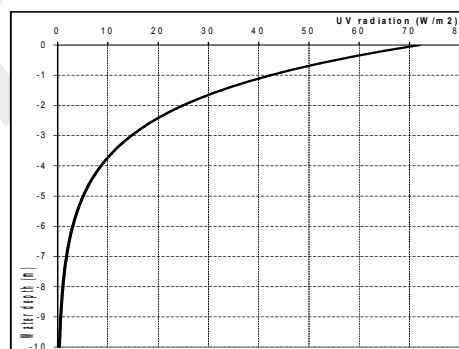
$$Mrt_{Cl} = k_{Cl} \times [Cl]$$

$$Mrt_{Rad} = Rc_{Rad} \times DL \times I \times f_{UV} \times \frac{1 - e^{(-Ext_{UV} \times H)}}{Ext_{UV} \times H}$$

| 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. | – |

| Input item | Description | Unit | Default value | Editable | Range |
|----------------|---|--|-----------------------------|----------|-----------------------------|
| I | solar radiation at segment upper boundary | W.m^{-2} | <i>derived from process</i> | n.a. | — |
| k_{Cl} | chloride related mortality constant | $\text{m}^3.\text{g}^{-1}.\text{d}^{-1}$ | $1.1 \cdot 10^{-5}$ | no | — |
| Mrt_{Cl} | chloride dependent mortality rate | d^{-1} | n.a. | n.a. | — |
| Mrt_{Rad} | radiation dependent mortality rate | d^{-1} | n.a. | n.a. | — |
| $Mrt_{E.Coli}$ | total mortality rate of <i>E.Coli</i> | d^{-1} | n.a. | n.a. | — |
| Rc_0 | first order mortality rate | d^{-1} | 0.8 | yes | 0.8 - 5.0 |
| Rc_{Rad} | radiation related mortality constant | $\text{m}^2.\text{W}^{-1}.\text{d}^{-1}$ | 0.086 | no | — |
| ϑ | temperature coefficient of the mortality rate | — | 1.07 | no | — |
| T | temperature | $^{\circ}\text{C}$ | 15 | yes | depends on local conditions |
| $[Cl]$ | chloride concentration | g.m^{-3} | <i>derived from process</i> | 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 | $\text{m}^2.\text{g}$ | 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 |

| Input item | Description | Unit | Default value | Editable | Range |
|------------|---|-------------------|---------------|----------|-------|
| I | solar radiation at segment upper boundary | W.m^{-2} | n.a. | n.a. | – |
| H | water depth | m | n.a. | n.a. | – |

B.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.

B.3.5 Output items

Apart from the concentration of the state variables, the following parameters are available as extra output:

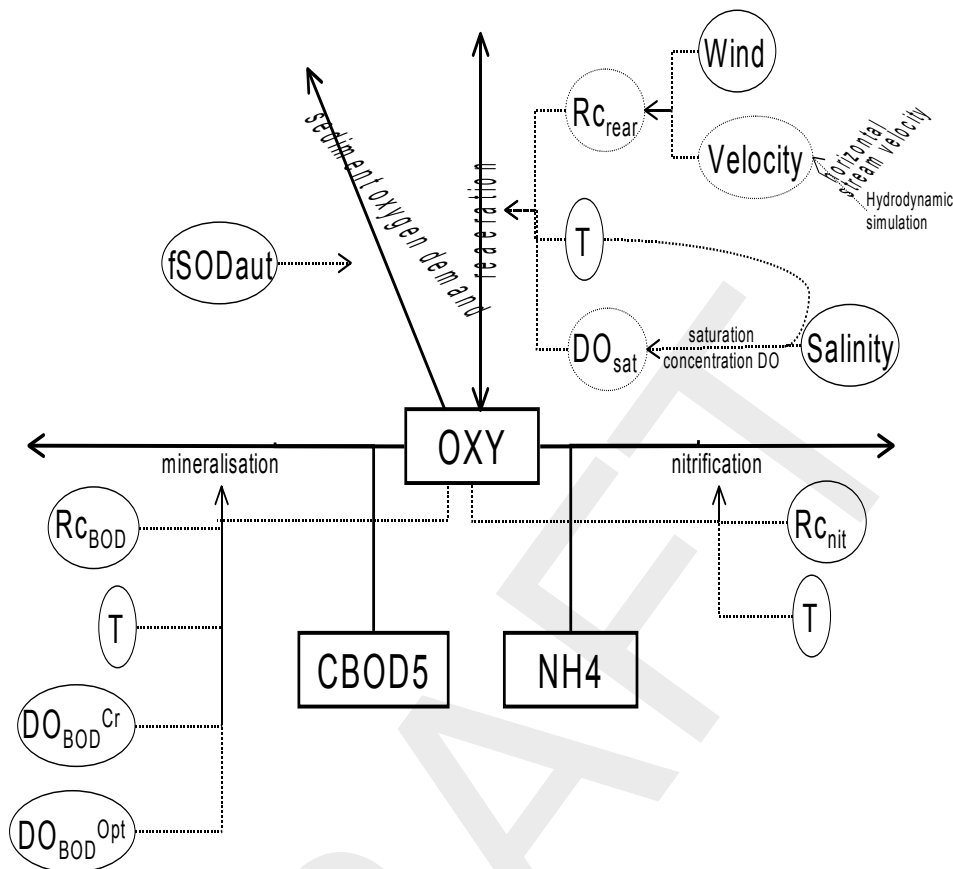
| Parameter id | Description | Unit | Model name |
|--------------|---------------------------------------|-----------------|------------|
| Ext_{UV} | total extinction of UV-radiation | m^{-1} | ExtUV |
| $MrtE.Coli$ | total mortality rate of <i>E.Coli</i> | d^{-1} | MrtToEColi |

B.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> |

General Dissolved Oxygen Model



B.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 | | | |

B.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:

$$\text{Mineralisation flux} = -R_{CBOD} \times [CBOD5] \times \vartheta_{BOD}^{(T-20)} \times \frac{[O_2] - DO_{BOD}^{Cr}}{DO_{BOD}^{Opt} - DO_{BOD}^{Cr}} \quad (\text{B.3})$$

| 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:

$$\text{Nitrification flux} = -R_{nit} \times [NH_4] \times \vartheta_{nit}^{(T-20)} \times \frac{[O_2] - DO_{nit}^{Cr}}{DO_{nit}^{Opt} - DO_{nit}^{Cr}} \quad (\text{B.5})$$

| Input item | Description | Unit | Default value | Editable | Range |
|-------------------|--|---------------|-----------------------|----------|-----------------------------|
| $[NH_4]$ | Concentration of ammonium | $gN.m^{-3}$ | n.a. (state variable) | n.a. | – |
| Rc_{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 |
| DO_{nit}^{Opt} | Optimal dissolved oxygen concentration for BOD mineralisation | $gO_2.m^{-3}$ | 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:

$$Reaeration\ flux = Rc_{rear} \times (DO_{sat} - [O_2]) \times \vartheta_{rear}^{(T-20)} \quad (B.6)$$

$$Rc_{rear} = f(\text{wind speed, stream velocity, water depth}) = f(Sw_{rear}) \quad (B.7)$$

$$DO_{sat} = f(T, \text{salinity}) \quad (B.8)$$

| Input item | Description | Unit | Default value | Editable | Range |
|--------------------|--|---------------|--------------------------|----------|-----------------------------|
| Rc_{rear} | First order reaeration rate constant | d^{-1} | n.a. (internal variable) | n.a. | – |
| DO_{sat} | Saturation concentration of dissolved oxygen | $gO_2.m^{-3}$ | derived from process | n.a. | – |
| $[O_2]$ | Dissolved oxygen concentration | $gO_2.m^{-3}$ | 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-WAQ, 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 $\text{g.m}^{-2}.\text{d}^{-1}$. 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.

B.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

B.4.4 Output items

Apart from the state variables, the following parameters are available as extra output:

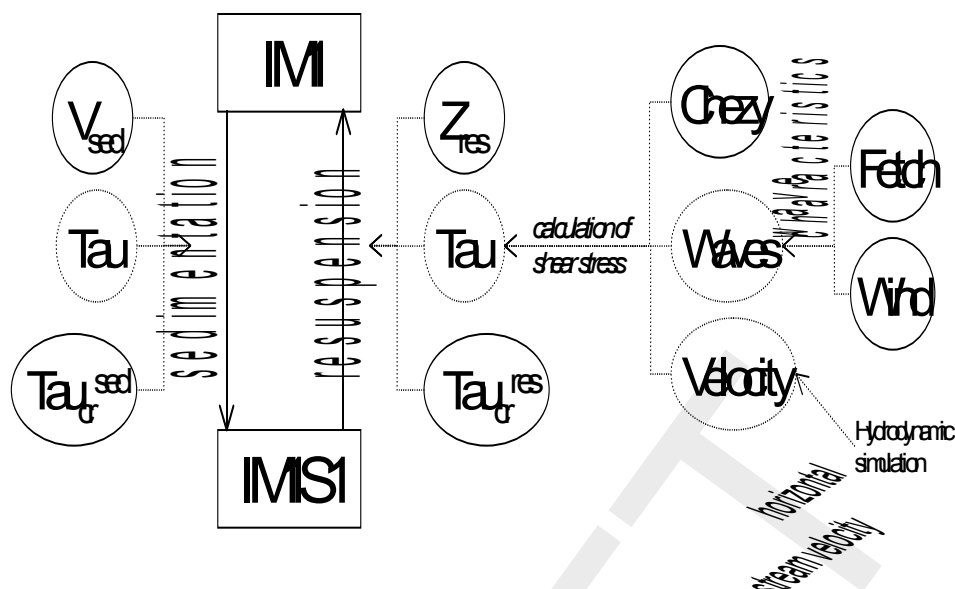
| Parameter id | Description | Unit | Model name |
|-----------------------------|--|-----------------------------|------------|
| R_{Crear} | Reaeration rate constant | d^{-1} | RCREAR |
| DO saturation percentage | Saturation percentage of dissolved oxygen | % | SatPercOXY |
| DO saturation concentration | Saturation concentration of dissolved oxygen | $\text{gO}_2.\text{m}^{-3}$ | SaturOXY |
| Stream velocity | Horizontal stream velocity | m.s^{-1} | Velocity |

B.5 Basic suspended sediment model

B.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> |



B.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 seaways 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-WAQ 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) Inorganic Matter in the sediment (settled) | IM1 IM1S1 | Sedimentation 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 | | | |

B.5.3 Description of processes

For a formal description refer to the Technical Reference Manual ([D-WAQ TRM, 2013](#)) for the individual processes of the Processes Library.

B.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-WAQ.

The sedimentation of $IM1$ depends on the ambient shear stress (Tau) and a user-defined critical shear stress for sedimentation (Tau_{cr}^{sed}). Only if the ambient shear stress is lower than the critical shear stress for sedimentation, sedimentation occurs:

$$Sedimentation\ flux = P_{sed} \times V_{sed} \times [IM1] \quad (B.9)$$

$$P_{sed} = \max \left(0, 1 - \frac{Tau}{Tau_{cr}^{sed}} \right) \quad (B.10)$$

| 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 | Ambient 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 ambient shear stress and a user-defined critical shear stress for resuspension (Tau_{cr}^{res}). Only if the ambient shear stress is higher than the critical shear

stress for resuspension, resuspension occurs:

$$Resuspension\ flux = P_{res} \times Z_{res} \quad (B.11)$$

$$P_{res} = \max \left(0, \frac{Tau_{cr}^{res}}{Tau} - 1 \right) \quad (B.12)$$

| 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 | $g\ m^{-2}\ d^{-1}$ | 0 | yes | 100 – 100,000 |
| Tau | Ambient 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 $100\ g\ m^{-2}\ d^{-1}$, then the resuspension flux of *IM1S1* is $10\ g\ m^{-2}\ d^{-1}$). These fractions are calculated by the process 'Composition of sediment layer S1'.

The ambient shear stress, Tau , represents the force exerted on the sediment by flowing water and wave action.

$$Tau = Tau_{veloc} + Tau_{waves} \quad (B.13)$$

$$Tau_{veloc} = f(\text{stream velocity, Chezy}) \quad (B.14)$$

$$Tau_{waves} = f(\text{wind speed, water depth, Fetch}) \quad (B.15)$$

| 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 | $m^{1/2}\ s^{-1}$ | 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 an 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).

$$Secchi\ Depth = \frac{PA_{constant}}{Ext_{VI}} \quad (B.16)$$

$$Ext_{VI} = Ext_{VI}^{Bak} + Ext_{VI}^{IM1} \times (IM1) \quad (B.17)$$

| 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 <i>IM1</i> | $m^2\ g^{-1}$ | 0.01 | yes | 0.01 – 0.05 |
| [<i>IM1</i>] | Concentration of Inorganic Matter 1 | $g\ m^{-3}$ | n.a. (state variable) | n.a. | — |

B.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.

B.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 |
|--------------------|-----------------------------------|---------------------|------------|
| τ | Ambient shear stress | $N\ m^{-2}$ | Tau |
| Sedimentation flux | Sedimentation flux of <i>IM1</i> | $g\ m^{-2}\ d^{-1}$ | fSedIM1 |
| Resuspension flux | Total resuspension flux | $g\ m^{-2}\ d^{-1}$ | fResS1DM |
| Ext_{VI} | Total extinction of Visible light | m^{-1} | ExtVL |
| Secchi Depth | Secchi disk depth | m | SecchiDept |
| Stream velocity | Horizontal stream velocity | $m\ s^{-1}$ | Velocity |

B.6 References

The references used in this appendix are:

- section B.3: Thomann and Mueller (1987)
- section B.4: Streeter and Phelps (1925)
- section B.5: Krone (1962); Partheniades (1962); Poole and Atkins (1929)

C Statistical output functions

D-WAQ offers a number of statistical output facilities as described in Chapter 5. 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 |

C.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

C.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.

C.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

C.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).

C.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

| Bucket | Number of values | Cumulative number |
|--------|------------------|-------------------|
| <1 | 10 | 10 |
| 1–2 | 20 | 30 |
| 2–3 | 20 | 50 |
| 3–4 | 20 | 70 |
| >4 | 10 | 80 |

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).

C.6 Percentage exceedance (*staprc*)

The *staprc* function enables you to compute the percentage of the time that a particular threshold 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 threshold is exceeded is computed.

Options:

threshold: The value 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 threshold ("no").

DRAFT

D Command-line arguments

D.1 Command-line arguments for the user-interface

With a few simple command-line arguments it is possible to automate important parts of the user-interface:

- ◇ Select a (new) hydrodynamic description file
- ◇ Select a (new) substances file
- ◇ Save the imported data into a (new) file
- ◇ Exit the program automatically

The following options are available:

| | | |
|--------------------|-----------------------|--|
| -coupling -comfile | <com-filename> | open the given communication file |
| -hydfile | <hyd-filename> | open the given hydrodynamic description file |
| -substances | <substances filename> | load the given substances file |
| -saveas | <new scenario file> | save the data under the given name |
| -save | | save the data under the same name (provided there is one) |
| -times | | start, stop and increment time in the following format, <code>yyyymmddhhmmss</code> (ex. "20110101070000 20110102070000 00000000010000") |
| -exit | | exit the user-interface (by itself it causes no saving of data!) |

These have to be handled in a sensible order (-exit last for instance!). For D-WAQ this means:

| | |
|-------------------------|---|
| -scenario | is treated first (if given; existing functionality) |
| -hydfile or -substances | can be done then |
| -save or -saveas | are handled thirdly |
| -exit | comes last |

D.2 Command-line arguments for the computational core

To run Delft3D-WAQ you need to use one or more command-line arguments. These are explained below. The basic invocation of the computational core is:

Preprocessing part:

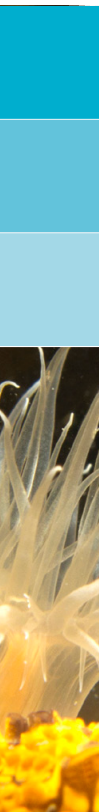
```
delwaq1 <input file> (one or more standard options ...)
```

and the computational part:

```
delwaq2 <input file> (zero or more specific options for the processes library ...)
```

The options for delwaq1 are:

- p <process definition file>: Specify the exact name of the process definition file (this is usually the standard file)



-waq, -eco, -chem Enable the water quality processes belonging to a particular module.

The options for delwaq2 are:

-openpb <process definition file>: Specify the exact name of the process definition file produced via the Open Processes Library Tool.

-nothreads <number> Turn on running in parallel on <number> threads. This will override any settings in the inp-file. Setting <number> to 0 or omission of <number> will run delwaq2 on all available threads.

Note that the first argument can be the name of the input file and that normally you do not need to give any other command-line arguments to the second program, delwaq2.

To accommodate a peculiarity that arises in the open processes library (which is compiled and linked into a DLL or shared object), the routine to retrieve a command-line option (`getcom()`) also reads from a file called `delwaq.options` in the current directory. The structure of that file is simple: each command-line argument must appear on a separate line, even if it is the value for another one.

Delft3D-WAQ also has a number of specialised options. They are mentioned here, but be aware that they should be used in a special context only:

-i <name of ini-file>: Use an INI file to specify what kind of submodel is to be used, the location of the processes definition file and other options.

-d Turn on domain decomposition mode, that is, get boundary conditions from other D-Water Quality processes

-m <value> Monitoring level - provide more or less output, depending on the value (defaults to 10)

-a Use only those water quality processes that are explicitly turned on

-np No processes are turned on at all

-conf <configuration> Specify the exact configuration (see also the options -waq, -eco and -chem above). The argument <configuration> must be a valid configuration.

-imax, -rmax, -cmax
<number> Reserve a larger array for processing the input – the array of integers (-imax), the array of reals (-rmax) or the array of strings (-cmax). If the preprocessor runs into problems with the available memory, it will report the sizes it requires. Rerunning the preprocessor step with one or more of these options will enable it to reserve the memory it requires.

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.

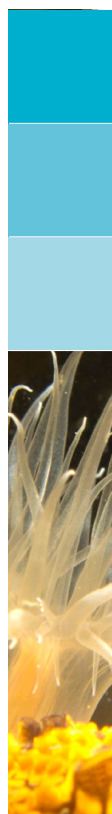
This appendix describes how that works and it also provides an example. The example that we provide is exactly the in-house Deltares implementation of the intake-outlet feature, but now in this new way. So, if you follow this appendix and compile the example application, then you get the standard Deltares 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 noseq

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,noseq)

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%segr`.

◇ **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} m³/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%segnr` 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 'inlout1.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 , nosege      , &
                                     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                :: nosege              ! number of segments
integer                :: itime                ! system time
real                   :: conc(notot,nosege)  ! 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
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
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%segr
    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 <inlout1.dat>')
2005 format (' error : number of combinations exceed maximum:',i4)
2006 format (' no file <inlout1.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
```


DRAFT

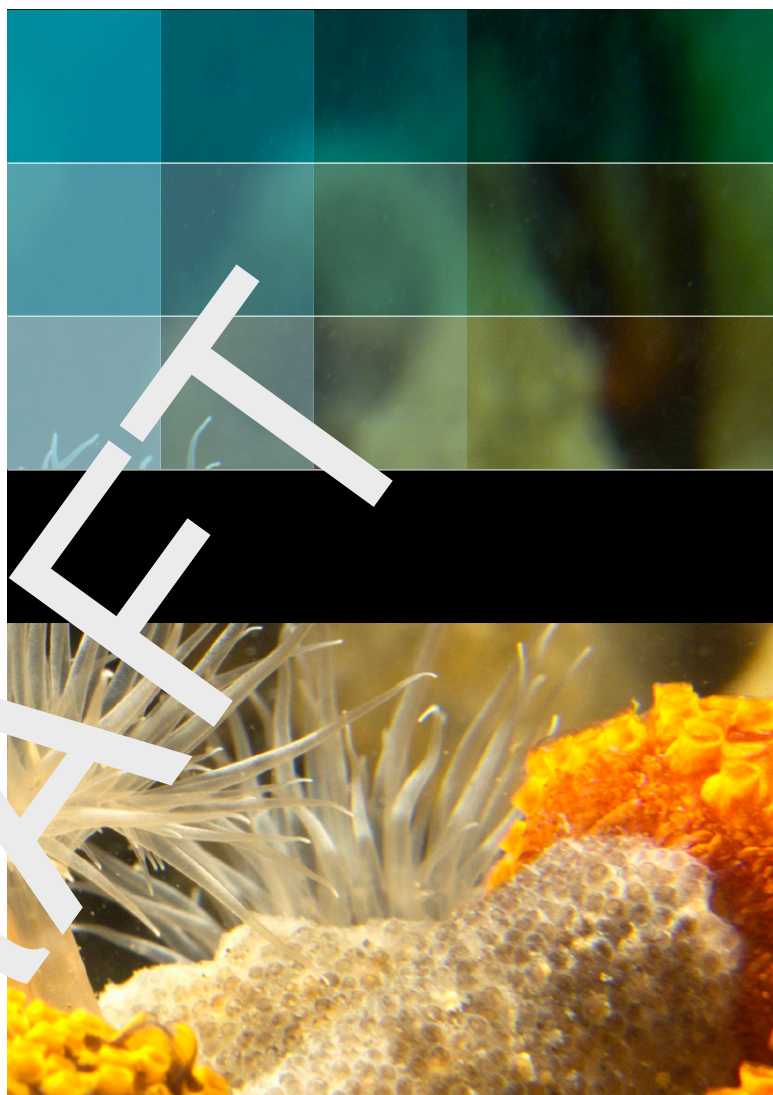


Photo by: Mathilde Matthijsse, www.zeelandonderwater.nl

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