Simulation software for safe, sustainable and future deltas

Delft3D FM Suite 2D3D

Deltares systems

D-Water Quality Input File Description

Technical Reference Manual

Deltares

D-Water Quality

Documentation of the input file

User Manual

Released for:
  Delft3D FM Suite 2023
  D-HYDRO Suite 2023
  SOBEK Suite 3.7
  WAQ Suite 2023

Version: 1.1
Revision: 78713

25 April 2024

D-Water Quality, User Manual

Published and printed by:

Deltares	telephone: +31 88 335 82 73
Boussinesqweg 1	e-mail: Information
2629 HV Delft	www: Deltares
P.O. 177	
2600 MH Delft	
The Netherlands	

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

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

Contents

List of Tables

0 A guide to this manual

0.1 Introduction

D-Water Quality is a generic mathematical model for water quality and ecology. It has two different parts that work together. It solves the equations for advective and diffusive transport of substances in water on the one hand and it models the water quality kinetics of chemistry, biology and physics that influence the behavior of substances and organisms in the water on the other hand. D-Water Quality is generally applied in waterflow of surface water and or ground water in any dimension, 1D, 2D-vertical, 2D-horizontal or 3D or a combination of these dimensionalities. Since it is strictly mass conserving with regard to both the transport of substance and the biological en chemical transformations between substances and organisms, it can be applied to compressible flows (like air) as well and a small number of these applications are known in the past decades. The vaste majority of applications however is in incompressible flow like water.

D-Water Quality does not compute the flow itself. It is connected to hydrodynamic flow models to obtain the likely flows in real life situations. Alternatively you may specify a stylistic flow field by hand yourself. D-Water Quality has been connected to the flow models Delft1D-2D (SOBEK), Delft2D-3D, Delft-FM, Simona and Waqua and to ROMS, TELEMAC 2D and 3D, Untrim, ECOM and ShyFem. Because of its mass conserving Finite Volume principles it can be connected to any water flow model that conserves mass. The mentioned models illustrate this. They range from Finite Difference models through Finite Volume models to Finite Element models both on structured and unstructured grids and with different dimensionality
This User Manual concerns the ASCII input processor. With this manual, the user should be able to make an ASCII input file that 'works'. Additional to this ASCII input, also the hydrodynamic flow data needs to be present. This is generally done by a coupling program that may be built into the hydrodynamic model like for Delft1D-2D (SOBEK), Delft2D-3D, Delft-FM, TELEMAC 2D and 3D and Untrim or that works on the output files of such a model. The coupling may act on single time steps, calling D-Water Quality as a dynamic link library (dll) or as a shared library per time step or the coupling may act on finished hydrodynamic results for subsequent multiple water quality model computations. The Deltares staff supports the construction of these coupling programs for any mass conserving third party flow model.

Although the manual will allow you to make a D-Water Quality ASCII input file to let the model 'work', it is generally convenient to have a correct sample input file at hand to start with. Such sample input files are produced by the Graphical User Interfaces that support the connection with many of the mentioned hydrodynamic modelling systems. The sample input file can then be modified according to your needs using this manual. This is especially valuable for those options that are not supported by the GUI yet. A **warning** should be given here: the input file that is described here is generally the output file of the GUI. This means that your modifications generally do not enter into the GUI again and any modified ASCII file will generally be overwritten by the GUI if you do not make the precaution to store it in a safe place and/or under a safe name.

The ASCII input file of the D-Water Quality model can be created and/or modified using a normal text editor. Be aware however that the D-Water Quality input processor may not understand tabs and word processor directives. The ASCII input of the D-Water Quality model is divided into 10 sections that are also distinguishable in the input file itself by section separation lines. Each section is called an input "group" and each input group is described in a separate chapter of this manual. Each input group closes with the token: #n, with n the group number. This closing token may start anywhere on a line like:

```
#4      ;  this is the end of group 4
```

If D-Water Quality does not encounter the closing token at the right location in the file, it will

produce an error. A summary of the subdivision into groups is given in Table 1.

Table 1: *Groups of ASCII input data for the D-Water Quality input processor*

Group	Description
1	identification, substance IDs
2	integration options, timers, monitoring
3	cells, grids, cell properties, volumes
4	exchanges, dispersions, velocities, flows, areas, lengthes
5	open boundary conditions
6	discharges and withdrawals
7	water quality constants, parameters, functions
8	initial conditions
9	output specification
10	statistical output

0.2 How to use this manual

Editing and modification of the input file is about the last step in a whole sequence of steps to set before you can do a water quality model simulation. We assume here that you have set the following steps before you arrive at the point that this manual becomes useful for you:

1 Make a set water flow files for water quality simulations with one of the supported hydro-dynamic models.
2 Import this hydrodynamics into the user interface and generate a simulation with default substance settings. This step should make an input file for a simulation with 1 substance 'continuity' with initial conditions and open boundary conditions of 1.0. Check that also waste loads with water flow associated with it should have a concentration of 1.0 attached to the water flow. Choose a safe integration option like option 15. Out should come 1.0. This proofs the mass conservation of the underlying hydrodynamics. Deviations may occur due to precipitation and evaporation that will likely not be included in your first test simulations.
3 Decide on the substances and processes to model. Try to select them through the PLCT (Process Library Control Tool). This tool produces a .sub file with the selected settings. Import this .sub file into the user interface.
4 Decide on the initial conditions, waste loads, coefficients that have no default value and decide on the most informative output for your selection.
5 Created a ASCII .inp input file and run the first and second step and make graphs of the results. This should give no significant problems, at least no problems where you need this manual for.
6 Modify your input and test alternative settings using this procedure. If you can complete your job in this way, then that is fine and you do not need this manual further more, since the GUI does everything for you.

7 Should you need functionality that is not supported by the GUI, then you may edit the .inp file manually to use that functionality. That is where this manual comes in.

8 Be aware that you have to save your manually edited file under a different name and / or at a different location the ensure that the GUI will not overwrite your edited input file. You may nevertheless use the GUI to run the D-Water Quality model with your edited input file. That saves you the trouble of determining the command line options to use.

9 You may easily make errors by manually editing your input file. You can inspect the correct interpretation of your input file by scanning the .lst output file. Search for strings like 'WARNING' or 'ERROR' if you find the .lst file too bulky to read it in detail.

0.3 Glossary

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

Substance	A D-Water Quality state variable. D-Water Quality models the transport of active or transported substances by solving the advection-diffusion equation numerically. The concentration of inactive or passive substances is not affected by advective or dispersive transport but only by the water quality processes. The D-Water Quality processes-library contains water quality processes and additional transport processes. The concentration of both the transported and the passive substances can be affected by the water quality processes.
Active (substance)	Active or transported substances are substances that will be transported by the flow of water, they thus consist of dissolved and particulate material in the water column.
Inactive (substance)	Inactive or passive substances are substances that are not transported by the flow of water. Substances that are part of the water bed or are attached to the water bed are passive substances.
Process	Processes are kinetic formulations that apply to substances. They can be divided into water quality processes and transport processes. A water quality process is associated with the transformation of substances into other substances (e.g. nitrification or mineralization) and it generates one or more *fluxes* between those substances. A transport process is associated with the redistribution of substances and it generates one or more *velocities* or *dispersions* additional to those already present by the movement of the water. Common transport processes are e.g. the sedimentation of particulates or additional dispersive transport of e.g. fish by own swimming. A process may also generate *process output*. Some processes only calculate process output, e.g. the calculation of the extinction of light. Other processes also calculate fluxes between substances.
Process output	Process output can be made available for post processing in the same way as the *substances* are displayed in graphs and numerical output files. This is very helpful to identify the value of intermediate variables like available light at a certain water depth or the sum of all modeled algae expressed as chlorophyll.
Flux	Many processes also compute fluxes as output. A flux is a change of the mass of a substance per unit of time and of volume as a result of the specific water quality *process* (for example the nitrification flux

	is the mass of ammonium converted to nitrate per unit of time and per unit of volume).
Segment	A segment indicates a D-Water Quality computational volume. D-Water Quality assumes that the model area is subdivided completely and non-overlapping in computational volumes (the Finite Volume Method). The word "volume" is also used for the volume in m^3 of a segment, so it is preferred to have different wording to avoid ambiguity.
Exchange	The complete subdivision of the model area into volumes has as consequence that adjacent volumes share an interface or exchange area through which flow and mixing takes place between those adjacent volumes. This is called *an exchange* and is defined by the *to* and *from* volume number on both sides. Positive flow is from the *from* volume to the *to* volume. Some numerical schemes also require a *from-minus-1* and a *to-plus-1* cell or volume number to allow for higher order accurate numerics.
Segment related and exchange related information	*Process input* and *process output* is divided into segment/volume related and exchange related information. Segment related information is defined for each *segment* of the schematization (e.g. parameters or concentrations). Exchange related information is known for each *exchange area* of the schematization (e.g. flows or additional velocities).
Exchange area	The contact surface of two linked computational volumes (or *segments*).
Constant	Input parameter that does not vary in time or in space.
Parameter	Spatially distributed input parameter that does not vary over time.
Function	Time variable function that does not vary spatially.
Segment function	Spatially distributed time function (usually a large and binary file created by other software) that contains information for a spatially distributed model parameter that varies over time.
Solver	Part of the computational core that solves the Advection Diffusion Equation (ADE)

0.4 Conventions for the input file

We did our best to make the D-Water Quality input file as flexible as possible and allow for a markup that is as readable as possible. You are kindly invited to signal if you see additional ways of improvement.

0.4.1 Markup options

The D-Water Quality input file is completely free formatted. This means that it does not matter how you make your layout of the input file. There is however one important restriction. You should specify your input in a fixed sequential order. This seems a limitation but you will notice that it on the contrary enhances convenience. You need not specify `<keyword>...<end-keyword>` sequences, or even nested versions of these sequences. Such constructions would have been necessary if the order was completely free because D-Water Quality should in one way or another understand what you want. D-Water Quality can now conclude intelligently from the sequence in your input, what options you are using.

The D-Water Quality input file with more or less this structure dates back to 1986 and old files are still read with minor or no adaptations with the present input processor. Unfortunately you still see some *option numbers* in the input file as remnants from this past. They function as switches and are not so clear. You need this manual to identify their meaning. Increasingly more we are changing those option numbers into meaningful keywords but we also want to remain compatible with older input files. So this manual aims to document the currently most modern version of the input processor and many of the outdated constructs are still supported, but are not explained in this manual any more.

The following markup rules are important:

◇ The ASCII input items are considered to be tokens separated by one or more spaces. This means that tokens containing spaces require special care. See under character input below.
◇ You must provide at the beginning of the file among others a *comment character*. This character indicates that everything that follows the character on the same line is a comment. You can use a comment line as header for the lines that follow as a kind of column headers. You can also continue information with a comment on the same line to indicate what the row is meant for.
◇ You may insert any amount of blank lines you need for readability.
◇ Character input like names/IDs can be inserted in the file without further quotes or double quotes. Only if the character string contains embedded blanks, it should be surrounded by single or double quotes. A string variable surrounded by single quotes may contain double quotes. A string variable surrounded by double quotes may contain single quotes. A string variable surrounded by any quotes may contain comment characters.
◇ Integers consist of numbers 0-9 only, optionally directly preceded by a sign.
◇ Floating point variables may be specified e.g. as -23.48 or as $0.25E+04$ or as $3.14e2$.
◇ Any keywords to steer input processing are always required in `CAPITALS`.

0.4.2 Convenience options

◇ If you have to insert numerous equal data you may use e.g. `312*' '` to insert 312 blank strings or `856*-312.456E-02` to define 856 times the real value. It is important that no spaces are allowed in between the heading count, the * and the item to be repeated. This feature cannot be nested.
◇ If you have a bulky table, that you do not want to be contained in the input file, you can specify `INCLUDE d:\my_dir\my_file.dat` at the location where the table should be included. If you omit the full path D-Water Quality assumes that the file is in the current dirctory. You are also allowed to use relative paths.
◇ The `INCLUDE` directive works up to 6 levels deep, so an included file may also contain `INCLUDE` directives. You should be aware that for relative paths, the path of the main input file is the starting point.
◇ There are several levels of diagnostic output given in Table 2. Each level will print also the items of the levels with a lower rank number.

***Table 2:** Supported diagnostic output levels of the D-Water Quality input processor*

Level	Output
Level 0	only very basic output
Level 1	substance names
Level 2	grid layouts, dispersion IDs and fields, boundary types, waste load types, names of constants, parameters, functions, segment functions
Level 3	administration of monitoring locations, boundary link andministration, boundary names and IDs, boundary time lags, waste load names and IDs, specific information on cells where defaults are overridden
Level 4	any variable time step specification
Level 5	features per grid cell

1 Identification, selected substances

This is the first group in the input file. The following example of the input for this group is produced by the user interface and reads like:

```
200 132 ';'    ; width of input and output, comment

; Type of DELWAQ input file:
; DELWAQ_VERSION_4.91
; Option for printing the report: verbose
; PRINT_OUTPUT_OPTION_4

; first block: identification
'd3d-waq-test021: "Friesche zeegat" area'
'2-Dimensional; dry cells removed'
'with statistical output'
'T0: 1990.08.05 00:00:00 (scu =       1s)'

; substances file: bod-do.sub
; hydrodynamic file: E:\delft3d\testbank\d3d-waq-test001\input\com-f34.dat

  2  1    ; number of active and inactive substances

; Index  Name
     1 'OXY'
     2 'CBOD5'
     3 'SOD'

#1 ; delimiter for the first block
```

1.1 The first line

The first line of the D-Water Quality ASCII input file has a specific meaning. It is not parsed by the parser but it provides information to initialize the parser. It contains 3 items:

◇ Maximum line length in number of characters for this input file. Longer lines will be truncated. At the moment of this writing, this value is limited to 1000 characters.
◇ Line length of the diagnostic output file. Here only 2 valid numbers are possible: 80 or 132. Any other number will result in the use of 80.
◇ A comment character. User interfaces generally produce `';'` for this character, but the user is free to select an alternative character. Everything after this character on the same line will be interpreted as "comment" that will not influence processing. In the following chapters of this manual we will also use ';' as the comment-character.

A valid example for the first line is: 200   132   `';'`

1.2 Version number and output option

Next the whole file is scanned for the presence of two strings. The strings are recognized anywhere in the text, so also if they are not placed in group 1, but they are commonly placed around the top of the input file. **They should be placed after a comment character that is at least followed by one or more blanks**.

◇ DELWAQ_VERSION_4.91
The string is immediately followed by a version number. The version number is a real of at most 5 characters long. This real should be higher than or equal to 4.90 and indicates the current style input processing that was introduced in 1996. Older input formats are no longer supported and are therefore not described in this manual. More explicitly, the
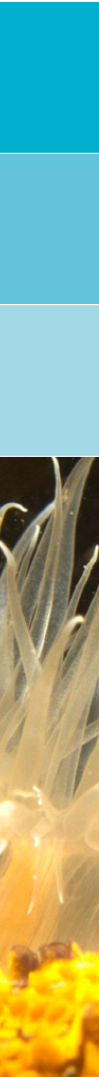
version number that corresponds with the contents of this manual is 4.91.

◇ `PRINT_OUTPUT_OPTION_4`

The string is immediately followed a 1 character integer that refers to the level of diagnostic output as was explained in table 2. The default output level is -1. This level, like level 0, only produces the most basic information.

1.3 Model title and calendar date string

The next input for the input processor should be 4 strings that form the model title. They are also displayed on printed output and in binary files. These strings should be present, so in case you do not want to use the option you have to provide e.g. `4*' '`. The strings are each 40 characters long. If longer strings are provided, they are truncated. In the example at the head of this chapter it can be seen that the strings may contain embedded comment characters and double quotes and blanks if surrounded by single quotes.

There are 2 different areas within these 4 title strings that have a special meaning:

◇ `MASS/M2`

If this token is present in the character positions 34-40 of the 3rd title string, then several programs assume that typical waterbed related substances are expressed in mass per m^2, rather than in mass per grid cell which was the unit before January 2011. You should not provide this information here. You should however be prepared that the D-Water Quality system overwrites the last 7 characters of your 3rd title string.

◇ `T0= 2006-06-21 18:05:00  (scu=       1s)`

This string is exactly 40 characters long. It is recognized if this is the 4th title string. It links the zero of the D-Water Quality internal timer to this absolute calendar time offset, and sets the basic unit of time.

The D-Water Quality internal timer is an integer. Theoretically this integer has the unit: 'system time'. This could be a second or a year or any other unit of time. All dimensions use this time further more, so if a year is chosen, then flow is expected as 'volume/year'. Implicitly most functionality assumes 1 second for the system time unit. models it may be useful to have a different unit of time than 1 second. That is why the presence of this 4th string gives opportunity to define a system timer (scu) in a number of seconds other than 1. The number is always in seconds, and is given in the 8 positions from position 31-38. You can also specify a system timer smaller than 1 second by a negative value. So -5 indicates $1/5^{th}$ of a second or 0.2 second and a value of -1000 indicates a millisecond. In general you will use however 1 second, like in the given example string.

The string upfront indicates the calendar date and time of the zero of the system time.

If the timer string is recognized, you can furthermore use absolute times in your input file. For output the system time is multiplied by the unit of system time in seconds (or divided if the value was negative) and then added to the calendar *zero* of the system time and then used for output of calender date and time of results.

CAUTION: As later will be discussed, the system time is a 32 bit signed integer at the moment, limiting the time span covered by the system time to plus or minus 64 years. This is likely to be changed in the near future, but has still to be anticipated by now. The calendar *zero* that you define here with the calendar time sting should be chosen sufficiently 'close' to the modeling interval to ensure that the whole modeling interval is contained in the interval of $\pm$ 64 years from the calendar time string.

If the timer string is not recognized, the times in input files are all expected in system time only and output times in output files are expressed in system time only.

1.4 Number of substances

D-Water Quality distinguishes substances that are transported with the water and substances that are passive. The latter are assumed to be attached to the water bed or to embankments. They are sometimes also called 'inactive', but that is probably not the right wording, since they are still subject to water quality processes. In the code of D-Water Quality the substances are called 'systems' and the amount of transported substances is called `NOSYS`. The total amount of substances is called `NOTOT`. The difference is the amount of passive substances. Input here may read like:

```
23       ; number of transported substances
 6       ; number of passive substances
```

Note: Because the passive substances are not transported, it is impossible to compute a steady state spatial concentration pattern due to stationary transport patterns for them. This is why passive substances are not allowed for the few steady state solvers within D-Water Quality. The relevant steady state solvers have numbers 17 and 18. The steady state solvers 6 - 9 are obsolete and should not be use any more.

1.5 Substance names

For each substance a name should be provided. A substance name is a string of 20 characters that serves as the ID of the substance. The substance name / ID should be unique. If a blank ' ' is given, D-Water Quality will make the name `Substance n` with n is the substance number.

The processes library recognizes substances from their ID, so the ID should correspond exactly with the corresponding ID in the processes library. Here the use of the the Graphical User Interface, GUI pays. Substances selected by the user interface enter into an input file created by the user interface automatically with the correct ID. It is nevertheless possible to add additional substances with different names. Because they are not recognized by the processes library, they are not subject to water quality processes, but they can e.g. be used as tracers in the model.

The sample input shows a sequence number and the substance ID. The user interface will make an input file with all substance IDs in order of the sequence number. You can change this order, by changing the sequence numbers. You are however not allowed to use the same sequence number twice and all passive substances should have the highest sequence numbers (the transported substances loop from 1 to `NOSYS` in the substances array, the passive substances loop from `NOSYS+1` to `NOTOT`). Input can look like:

```
      2         1    ; number of active and inactive substances
; Index       Name
      2         OXY      ; Oxygen in mg/l
      1         CBOD5    ; Carbonous BOD-5 in mg/l|
      3         SOD      ; Sediment oxygen demand in mg/m2
```

You will note how the comments are used to enhance readability of the data. You will also note that it does not matter whether the numbers of transported and passive substances are mentioned on one line or on different lines. It also does not matter where the information is placed on the line, only the order in which the information appears matters.

1.5.1 Multiple copies of substances

Up to the year 2011 D-Water Quality substances are specified like mentioned earlier. Increasingly more however the need came up to model several instances of a substance separately.

All these instances should basically share the same processes in the processes library, albeit with optionally different reaction coefficients. This could be done by just specifying their IDs like above, but that becomes less practical if 100 sediment fractions are required or 57 conservative tracers to monitor the fate from 57 waste fluxes or the specification of 50 algae species in mutual competition. For that reason a functionality has started to appear from 2011 on that is called *multiple substances*.

The input is simple:

```
    2           1              ; number of active and inactive substances
  ; Index      Name
    2           OXY            ; Oxygen in mg/l
    1           CBOD5 *5       ; 5 instances of CBOD5
    3           SOD *5         ; 5 instances of Suspended Sediments at the bed
```

Note:

◇ The passive substance at the water bed is the last substance.

◇ If 2 plus 1 substances are specified respectively then only for this three substances the ID's need to be specified.

◇ There should be a space between the ID and the '*n' token.

◇ There should be no space between '*' and the 1-3 digits that specify the amount.

◇ Due to the multiplication, $1 + 2*5 = 11$ substances are finally modeled, 5 of them are passive.

◇ The substances turn out to be automatically named CBOD501 - CBOD505 and SOD01 - SOD05.

◇ If two substances share fluxes and have the same multiplicity, then it is automatically assumed that the single substances with the same number are coupled.

1.6 Finalization

This part of the input file is finalized with the `#1` end of first data group indicator.

2 Timers, integration, monitoring

This is the second group in the input file. The input for this group may read like:

```
;       second block of model input (timers)

; factor   timer string    processes timer
  86400    'ddhhmmss'        'ddhhmmss'
   5.70   ; integration option 5, sub-options .70 ;
; detailed balance options
  BAL_NOLUMPPROCESSES
  BAL_NOLUMPLOADS
  BAL_NOLUMPTRANSPORT

;   ddhhmmss
   0123000       ; simulation start time
  25123000       ; simulation stop time
         0       ; constant time step
   0000500       ; time step size
;
         7       ; number of monitoring points/areas
;      name     n=    numbers
    '(3,14)'    1     208
    '(4,14)'    1     209
    '(12,8)'    1     110
    '(18,11)'   1     165
  '(7-8,5-6)'   4      57 58 73 74
    '(7,11)'    1     154
    '(11,2)'    1       8
         0       ; monitoring transects not used

;   start time      stop time      time step           of
;   ddhhmmss        ddhhmmss       ddhhmmss
    0123000        25123000        0123000       ; monitoring
    0123000        25123000        0123000       ; map, dump
    0123000        25123000        0003000       ; history

    #2 ; delimiter for the second block
```

2.1 Time factor and time strings

◇ **factor between timers**

D-Water Quality uses for its input processing 2 different timers. The first timer is de model timer and is specified as part of the 4th title string in the first group of the input file. It is usually set to 1 second. The second timer is the auxiliary timer that is used for water quality processes. This timer is generally expressed in days (a decay coefficient in 1/day). D-Water Quality supports freedom of choice in this respect, but it is not excluded that some processes routines lean on the fact that the processes timer is generally expressed in days. Because the unit of time is free, only the factor between the two timers need to be provided. This is generally 86400, the number of seconds in a day. Should you chose however a system time of days (and thus flows in m^3/day) and processes expressed per year, then you could take 365 as factor.

◇ **timer strings**

D-Water Quality timers are integers. This helps avoiding round-off errors. It is however more convenient to tell D-Water Quality that it has to stop simulation 'after 31 days', rather than 'after 2678400 seconds'. For this reason you may tell D-Water Quality that you will provide input in DDHHMMSS format. This allows you to specify 31000000 for 31 days. D-Water Quality is still using 32 bits signed integers for its timers and thus you may not specify a higher time then 2147 days 48 hours 36 minutes and 48 seconds, since 2147483648

equals 2^{31}. This limits your specification to 5 years and 10 month. This may change in near future, but you can in the mean time use the alternative of specifying times in YYDDDHH format for a maximum of 2^{31} seconds = slightly over 68 years. You must give a timer string for both the system timer and for the auxiliary (processes) timer. Your choice will hold for the time integers that you specify throughout the complete input file.

The times that you specify this way are in system time units. If you want to know where they are located on the calendar, then you have to add them to the reference time as mentioned in the reference time string. Please be aware that D-Water Quality assumes 365 days within one year of its system time units. The specification in system time units can thus mean a shift of a day per 4 years in the date and time that may be printed. This can be avoided. At many locations in the D-Water Quality input file you can alternatively provide a calendar string instead of an integer. This only works if you also did specify a reference time. D-Water Quality will then subtract the reference time and date from your specified time and date and use the result in seconds as the system time of you input. The following strings are valid timer strings:

- DDHHMMSS
- ddhhmmss
- YYDDDHH
- yydddhh
- ' '

The blank character indicates that just the system timer is used. If one timer string was set to DDHHMMSS, then only ' ' or DDHHMMSS are allowed for the other string. If one timer string was set to YYDDDHH, then only ' ' or YYDDDHH are allowed for the other string. So if both timer strings are not blank, they should be equal.

2.2 Integration procedure

The integration procedure consists of an integer. There are at the moment the following integration procedures:

◇ Option 0: no transport, just processes
◇ Option 1: backward in space and time
◇ Option 5: Flux corrected transport
◇ Option 6: Direct steady state, backward differences in space
◇ Option 7: Direct steady state, central differences in space
◇ Option 11: Horizontal explicit upwind, vertical implicit central
◇ Option 12: Horizontal explicit FCT , vertical implicit central
◇ Option 13: Horizontal explicit upwind, vertical implicit upwind
◇ Option 14: Horizontal explicit FCT , vertical implicit upwind
◇ Option 15: GMRES, horizontal upwind, vertical upwind
◇ Option 16: GMRES, horizontal upwind, vertical central
◇ Option 17: stationary GMRES, horizontal upwind, vertical upwind
◇ Option 18: stationary GMRES, horizontal upwind, vertical central
◇ Option 21: Self adjusting teta method (limiter Salezac)
◇ Option 22: Self adjusting teta method (limiter Boris and Book)
◇ Option 23: Leonards QUICKEST
◇ Option 24: Local flexible time step method by Leonard Postma

(The missing option numbers represent integration procedures that were removed, as they are not suitable for current-day model schematisations. Examples include dynamic, fully implicit methods that could only be applied in two-dimensional models or procedures requiring structured grids.)

You can select any of the above options. The D-Water Quality user manual indicates the technical specification of the integration procedures.

In older input files you may see the integration number be followed by a period and 1, 2 or 3 digits behind the period. The information behind the period indicated settings for keywords nr. 1 - 6 of table 2.1. It is advised to use those keywords furthermore, although the 3 digits are still supported. If you want to backtrack the used options in an older file, then the following rule applies:

⬦ if the first digit after the period

□ is 0, then none of the first three keywords is set.
□ is 1, then the first keyword is set.
□ is 2, then the second keyword is set.
□ is 3, then first and second keywords are set.
□ is 4, then the third keyword is set.
□ is 5, then first and third keywords are set.
□ is 6, then second and third keywords are set.
□ is 7, then all three first keywords are set.

⬦ if there are second and/or third digits after the period then, if they both:

□ form 01, then the fourth keyword is set.
□ form 11 or 20, then fourth and fifth keyword is set.
□ form 30, then fourth, fifth and sixth keywords are set.

2.3 Optional keywords

At this location a number of optional keywords are supported. They are listed in table 2.1.

Table 2.1: Supported keyword steered options in the D-Water Quality input processor

Number	Keyword	Description
1	NODISP-AT-NOFLOW DISP-AT-NOFLOW[a]	**No dispersion at zero flow** Useful to prevent dispersive fluxes towards dry cells and to prevent dispersion through thin dams.
2	NODISP-AT-BOUND DISP-AT-BOUND[a]	**No dispersion across open boundaries** Ensures a flux of concentration times flow at boundaries without additional dispersion term.
3	LOWER-ORDER-AT-BOUND HIGHER-ORDER-AT-BOUND[a]	**No flux correction at boundaries** Only relevant for higher order schemes, **very advisable**.
4	BALANCES-OLD-STYLE NO-BALANCES[a]	**Set balances to *on*** This triggers the output of balance information.
5	BALANCES-GPP-STYLE	**writes GPP style balances** Switches the SOBEK balances *off*.

Number	Keyword	Description
6	BALANCES-SOBEK-STYLE	**writes SOBEK style balances** Switches also the GPP balances *on*.
7	FORESTER NO-FORESTER[a]	**Switches the Forester monotony filter on** Only of relevance for schemes with central differences in the vertical.
8	ANTICREEP NO-ANTICREEP[a]	**Prevents artificial creep by diffusion** Only relevant with integration types 19 or 20 and sigma coordinates.
9	BAL_NOLUMPPROCESSES BAL_LUMPPROCESSES[a]	**Distinguishes all processes separately** Show all processes separately in the balances.
10	BAL_NOLUMPLOADS BAL_LUMPLOADS[a]	**Distinguishes all waste loads separately** Show all waste loads separately in the balances.
11	BAL_NOLUMPTRANSPORT BAL_LUMPTRANSPORT[a]	**Distinguishes fluxes separately** Show dispersive and advective fluxes separately in the balances.
12	BAL_UNITAREA	**Makes balances per** m^2
13	BAL_UNITVOLUME	**Makes balances per** m^3
14	BAL_NOSUPPRESSSPACE BAL_SUPPRESSSPACE[1]	To be documented.
15	BAL_NOSUPPRESSTIME BAL_SUPPRESSTIME[a]	To be documented.
16	SCHEME15_UNSTRUCTURED SCHEME15_STRUCTURED[a]	**3rd dimension not treated as layered** Also iterates the 3D model dimension rather than a simple double sweep inversion.
17	ANTIDIFFUSION NO-ANTIDIFFUSION[a]	**Option of scheme 21 and 22** To be documented.
18	PARTICLE_TRACKING	**Particle tracking within D-Water Quality**

From the table 2.1 it can be seen that often also the negations are generally recognized. They are of less importance, because they are the default setting. You may use as many of the keywords mentioned as you need and their order of appearance is generally not important.

---

[1]this is the default

Keywords 4, 5 and 6 are mutually exclusive like the two keywords that negate each other. In such a situation the last of the mutually exclusive keywords prevails.

2.3.1 Particle tracking

The `PARTICLE_TRACKING` functionality requires a filename as additional information. The filename should be the name of the so-called <∗.mdp> file that is described in the D-WAQ PART manual. The steps to be set to incorporate particle tracking into Delwaq are the following:

1 You set up a particle tracking simulation according to the specifications of the D-WAQ PART manual. This simulation is invoked either by the user interface or manually by you from the command line by the instruction `delpar.exe` *my-input-file*.mdp. You inspect this simulation for correct behavior.

2 You set up a D-Water Quality simulation and you take care that:

  ◇ You are using exactly the same hydrodynamic input files as you used for the particle tracking simulation.
  ◇ You are using exactly the same start time and stop time of simulation as you used for the particle tracking simulation.
  ◇ You are using exactly the same integration time step size as you used for the particle tracking simulation.

  The interface between D-Water Quality and D-WAQ PART will check this and produce error messages if one or more of the mentioned conditions are not fulfilled.

3 You enter the `PARTICLE_TRACKING` keyword followed by the name of your <.mdp> file in the D-Water Quality input file. You will then note that D-Water Quality reads the particle input information and adds the D-WAQ PART substances as *passive substances* to the D-Water Quality simulation. You will also note that the remainder of the D-Water Quality input file can remain the same until the specification of the initial conditions.

4 You insert initial condition values for all D-WAQ PART substances in group 8 of the D-Water Quality input file. The most obvious value to enter is 0.0 here.

You will note that you can now run a joint D-Water Quality and D-WAQ PART simulation. You will also note that the D-WAQ PART substances appear in the monitoring file, the <.map> file and the <.his> file. Moreover, the D-Water Quality model concentrations are now available to the D-WAQ PART simulation and the D-WAQ PART model concentrations are available to the D-Water Quality water quality processes.

You may wonder why you should model some substances with a particle tracking model and other substances with a Finite volume advection- diffusion solver in D-Water Quality. The reason is that the grid cell, the Finite Volume, is the smallest unit that D-Water Quality distinguishes. If you are using a grid that is not so fine, then point sources will spread immediately over the grid cell, whereas in reality it might take up to a day before an initially released patch of dye has grown sufficiently large that the Finite Volume ADE solver can take over the computation of the result. To avoid an unrealistic initial spreading you may consider to model the initial spreading process using the particle tracking option and continue the modeling afterwards using the Finite Volume solver. For this aim the D-Water Quality take over time or delay time that was mentioned in the D-WAQ PART manual as "no longer being supported" is revived again. That works as follows:

◇ If you name a substance in the D-WAQ PART part of the simulation exactly identical to a corresponding substance in the D-Water Quality part of the simulation, but with an additional 'p' just behind the D-Water Quality name, then the interface between both knows that these two substances belong to each other.

◇ If you specify a D-Water Quality take over time, generally in the orde of 1 day, in the D-

WAQ PART input file, then all particles that did stay longer than the specified take over time span in D-WAQ PART are removed from the D-WAQ PART simulation and are migrated towards the D-Water Quality simulation as a contribution to the concentration in the grid cell where they were. D-Water Quality will transport this mass further with its Finite Volume solvers.

◇ If you add both results, you will see the advantage of the efficient and robust mid-field and far-field modeling with D-Water Quality and you will note the sub grid patch and concentration patterns that are modeled with D-WAQ PART for the initial period just after release.

This is just one example of the benefits of the joint simulation of D-Water Quality and D-WAQ PART. Other examples are:

◇ model spilled oil patches with D-WAQ PART and let the entrained and emulgated oil migrate from the D-WAQ PART side to the D-Water Quality side and use the results there to identify the exposure of sensitive receivers like fish and coral reefs to the dispersed oil fractions.
◇ use the D-WAQ PART 'time in the system' variable per particle to determine the shift from fish eggs to larvae and juvenile species and let the thus modeled species get their food from the concentration of algae, zooplankton or other particulate organic carbon that is modeled by D-Water Quality.

2.4 Integration timers

The D-Water Quality input processor now expects the integration timers:

◇ The start time of integration
◇ The stop time of integration
  The start and stop times can either appear as an integer in system units or in DDHHMMSS style or in YYDDDHH style. This is then taken as the time in system units after the calendar offset string if that was present.
  Alternatively the start and stop times can be specified as a calendar time string e.g:

$$2010/07/31-12:00:00$$

  Please be aware that an error is generated even if you only use other separation characters between the digits of the date. The parser is very strict.
◇ The time step option switch.
  There are 2 values allowed:

  0 indicating a constant time step size
  1 indicating a time varying time step size

◇ The information on the time step of the integration

  ▫ In the case of a constant, an integer is required in system units or in DDHHMMSS style or in YYDDDHH style.
  ▫ In the case of a time series the following information is expected:

    ○ A positive integer indication the number of time function breakpoints
    ○ That many pairs of time integers. The first is the breakpoint time and the second is the size of the time step at that breakpoint. The 2 integers are either in units of the system clock or in DDHHMMSS style or in YYDDDHH style.

  The breakpoint times should be positive and in increasing order. At the breakpoint time the time step size changes to the value that was specified for the breakpoint. It is the responsibility of the user to choose the breakpoint times such that it is clear when the time step size changes (the prescribed time may not be the start time of a new time step) and to specify time step values in such a way that the output times, that are

specified later on, do not conflict with the way this time series is established.

Because of these associated problems, a variable time step size is hardly used in D-Water Quality but it should work correctly.

2.5 Monitoring locations and monitoring transects

Once D-Water Quality produces concentrations of substances throughout the area, flexible ways for presentation of these results are required. One way is to make time series, generally with high frequency, of the values at a certain location or through a certain transect. Input required is:

◇ an integer to indicate if monitoring areas are used: 1 means "yes", 0 means "no".

◇ the integer total number of **monitoring areas**

Monitoring locations can consist of a group of computational volumes, a so called *monitoring area*. The single monitoring location consisting of a single grid-cell is just a special case of the general monitoring area. Furthermore, if the output of balances was selected for the model, then they are automatically produced for all monitoring areas, unless explicitly switched off for specific areas.

If the number of monitoring areas is non zero, then that many sets of the following information is expected:

▫ a string with a meaningful name of the monitoring area. This string should be unique and if `' '` is provided, D-Water Quality makes `Observation-idnnn` as name.
▫ an optional string `NO_BALANCE` to indicate that this area should be excluded from the balances output.
▫ the integer number of volumes that form together this monitoring area.
▫ That many integer sequence numbers of the *computational volumes* that form together this area.

Note: The DIDO grid manipulation tool of the Graphical User Interface is able to make ASCII files with monitoring areas that can directly be included into the D-Water Quality input file. You may need to edit the file because it is using # as comment character while you may use `;`.

Note: 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
```

◇ an integer to indicate if monitoring transects are used: 1 means "yes", 0 means "no".

◇ the integer total number of **monitoring transects**
The input processing also allows for the specification of monitoring transects. A transect consists of a number of interface areas between *computational volumes*.
If the number is monitoring transects is not zero then that many sets of the following information is expected:

▫ a string with a meaningful name of the monitoring transect. This string should be unique and if ' ' is provided, D-Water Quality makes `Transect-idnnnnnn` as name.
▫ an integer option number to indicate how the transect information should be accumulated. This option number can have one of three values:

  1 the net fluxes will be displayed for the transect.
  2 only the sum of the positive fluxes through the transect will be displayed.
  3 only the sum of the negative fluxes through the transect will be displayed.

  The sign of the flux is relative to the 'from-' and 'to-' segment number of the exchange. To have both the positive and the negative fluxes displayed, mention the transect twice, once for the positive and once for the negative fluxes.
▫ the integer number of exchange surfaces that together form this monitoring transect.
▫ That many integer sequence numbers of the *exchange surfaces* that form this transect.

Note: Unfortunately the DIDO grid manipulation tool does not support monitoring transects. This may make it very tedious to specify transects, because you have no easy access to the values of the numbers of the interfaces between the different *computational volumes* if they are produced by a hydrodynamic model.

Here is a small example:

```
1 ; Use monitoring locations/areas
3 ; nr of monitor locations and areas
'ObsPoint 1' 1  ; Just a single segment
3548
'ObsPoint 2' 1  ; Just a single segment
4352
'ObsArea 1' 5   ; Use 5 consecutive segments
3891 3892 3893 3894 3895

1 ; Use monitoring transects
1 ; nr of monitoring transects
'Transect 1'  2  13  ; Select 13 exchange areas, use the positive fluxes (option 2)
     2943      9635      3322      3427      3532
     3637      3751      3872      3999      4133
     4268      4404     11126
```

2.6 Output timers

D-Water Quality has 3 output timers:

1 monitoring timer
The monitoring timer is used to write the monitoring file. The monitoring is a readible ASCII file that contains all relevant run-time messages and simulation result summaries including area-wide mass balances. If detail balances have been switched *on*, then the monitoring file also contains detail balance information. The monitoring timer indicates the

start time, stop time and time step to be used for these summary statistics and readible balance information.

2 map-file timer

The map-file timer steers the start time, stop time and time step of the binary map file. This file contains all desired output on the complete model grid. This can become large and that is why there is a separate map-file timer.

3 history timer

The history file also is a binary output file but only at the selected monitoring locations. That is why the history timer is generally selected to be more frequent than the ASCII monitoring

Each timer consists of 3 timer entries:

1 a start time
This can be an integer or a valid calendar time string
2 a stop time
This can be an integer or a valid calendar time string
3 a time step
This can only be an integer

It is the responsibility of the user to ensure that the output timers coincide with an integer multiple since start of simulation of the least common multiple of all transport and water quality time steps that are used. This is an integer multiple of the transport time step if that is used also for water quality. If (some) water quality processes are computed with a longer time step, then it is an integer multiple of the longer time step.

2.7 Finalization

This part of the input file is finalized with the #2 end of second data group indicator.

3 Grid and values of the volumes

This is the third group in the input file. The following example of the input is derived from a small model for an advisory project.

```
; third block of model input (grid layout)
      1430          ; number of segments
;
MULTIGRID

      INCLUDE       ../model-input/grid_layout.dat

END_MULTIGRID

       NONE               ; grid layout not used
;
; attributes
;
      INCLUDE '../hydro/hyd3g/com-hyd3g.atr'
;
; volumes
;
      -2              ; first volume option
      '../hydro/hyd3g/com-hyd3g.vol'
;
 #3             ; delimiter for the third block
```

3.1 UGRID grid specification (optional)

D-Water Quality used to produce two types of output files for history and map data: the plain binary files and the self-descriptive `NEFIS` files. Neither of these files contain any information on the shape of the grid. To visualise the results you always need an extra file or files that contain the grid information.

If you specify a *WAQGEOM* file, which is produced by various hydrodynamic models such as Delft3D-FLOW D-Flow FM or SOBEK. by means of the `UGRID` option in group 3, the model will write `NetCDF` map and history files. Be sure to switch on NEFIS/NetCDF output options in group 9.

The specification must be added at the start of this group:

```
; third block of model input (grid layout)
UGRID 'grid_waqgeom.nc'

      1430          ; number of segments (or a MULTIGRID specification instead)
      ...
 #3             ; delimiter for the third block
```

If the first word in this section is not `UGRID`, the option is skipped.

3.2 Number of computational volumes

The D-Water Quality Finite Volume Model assumes that the modeling area is subdivided into computational volumes. The subdivision should be complete (covering the whole model area) and non-overlapping. This is the location in the file to specify how many volumes are used. In the example input that are 1430 volumes or *segments*.
This is the *base grid*. The word *grid* suggests a systematic ordering of the computational

volumes. Although this ordering often exists, it is no requirement. A few of the D-Water Quality advection diffusion solvers require a matrix type of topology of the computational grid, but most allow a free ordering.

There is however one limitation. If the model is 3-dimensional, then D-Water Quality assumes that the first n computational volumes are located at the top and form the water surface with incoming solar radiation and with reaeration of oxygen and CO_2. D-Water Quality also assumes than the last computational volume number of a water column is located at the water bed and either interacts with the bed or features inactive substances laying on the bed. In between it is assumed that computational volumes that are lower in the water column have a higher sequence number. The vertical vector and numbering is positive in the downward direction. This is unlike many hydrodynamic models. The D-Water Quality preference stems from the convenience that the first n computational volumes describe the complete spatial coverage of the model. If we would have numbered the other way around then, in models with fixed layer depths, the first few wet computational volumes would contain the few deep cells in gullies and the full extent of the model area is only visible by inspection of the last n computational volumes, but where does this start in the array space?

3.3 Grid information

The *base grid* is the linear array of computational volumes of D-Water Quality. It is convenient to distinguish other grids as well. It can be useful to distinguish the segments just above the bed to give them bed related coefficients etc. It can also be useful to distinguish the segments at the water surface etc. Furthermore, the D-Water Quality model is not limited to the water phase, also a number of computational volumes in the bed can be distinguished. Often the schematization of cells in the bed can be much coarser than in the water column, because transport in the layered bed is assumed to be limited to vertical transport only.

In the optional `MULTIGRID` section of the input, you are able to define a number of additional grids and refer to them later on by their name. If the keyword is not used, then there is only one grid, the *base grid*. In our sample input file the `MULTIGRID` information is included from a file. That file contains e.g. the following information:

```
ZMODEL  NOLAY  13

   SUBGRID 'water-grid'
   INCLUDE '../model-input/water-grid-ag01.dwq'

   SUBGRID 'water-zone'    1430*1

   BOTTOMGRID 'sediment-grid'
   REFERENCEGRID 'Base grid'
   INCLUDE '../model-input/bottom-grid.dwq'

   BOTTOMGRID 'sediment-zone'
   REFERENCEGRID 'sediment-grid'  25*1  60*2   25*3

   BOTTOMGRID 'sediment-default'
   REFERENCEGRID 'sediment-zone' 3*1

   NOBOTTOMLAY INPUTGRID sediment-zone 10 8 5
```

At this location a number of optional keywords is supported. They are listed in table 3.1.

Table 3.1: Supported keywords in the grid information section

Keyword	Description
NOLAY[1]	The number of layers will follow as an integer. If absent D-Water Quality will try to infer the number of layers from other information.
	Should always be used before the definition of the additional grids
MULTIGRID	Starts the definition of multiple grids.
ZMODEL	The model has horizontal layers and the bed may be located in different layer positions at different horizontal locations.
SUBGRID	A sub-grid will be defined.
PROCESSGRID	A grid for processes will be defined.
	Both options are equivalent.
BOTTOMGRID	A grid for a layered sediment model will be defined
BEDGRID	Equivalent with BOTTOMGRID
NOBOTTOMLAY	The number of bed-layers will be read
BOTTOMGRID_FROM_ATTRIBUTES	Indicates the next information is an attributes file (see below)
SUBSTANCE_PROCESSGRID	A grid for substances and processes will be read
PROCESS_TIMESTEP_MULTIPLIER	A process time step multiplier will be read
END_MULTIGRID	Ends the definition of multiple grids

In the sample input file the model is defined to be a z-layer model, so it has horizontal layers at fixed depth. The number of layers is given as 13. It could be possible that D-Water Quality is able to identify the number of layers from its own, since the layers are full in this case (13 layers of 110 cells each). To avoid unambiguity it is good to define the number of layers here. Then 5 different grids are defined. Finally the numbers of layers in the bed are defined.

3.3.1 Definition of a grid

The definition of grids for different application (sub-grid, bed-grid, substance_process-grid) is basically the same. The new grid should have a grid where it bases on. This means that the first additional grid that is defined (the "water-grid" in this case) always *clones* the *base grid*. The grid definition then gives a sequence number to each grid cell entry of the grid that it *clones*. In our example the base grid has 1430 computational volumes. So a grid definition consists of 1430 numbers that tell how the new grid is mapped on the old grid. This means

---

[1]also allowed without MULTIGRID

that the new grid may be coarser than the old grid (have less cells, so the highest cell number then is lower than 1430 in our case), but can never be finer. Given the hydrodynamic grid as the *base grid*, the DIDO grid manipulation tool of the Graphical User Interface is able to make ASCII aggregation files that can directly be used in the D-Water Quality input file as grid mapping. You may need to edit the file because it is using # as comment character while you may use ; .

To define new grids, the following information is expected in exactly this order:

◇ A unique string with the name / ID of the additional gridindexGrid!ID that is created
◇ One of the following optional keywords:

  ▫ NOLAY followed by an integer.
    This specifies the number of layers in the grid that is created. If absent, D-Water Quality assumes that the new grid has as much layers as the grid it is referring to.
  ▫ REFERENCEGRID followed by an ID of an already created grid.
    The new grid will *clone* this *reference grid*. If absent the *base grid* will be used as the reference grid for this new grid.

◇ The mapping data from the reference grid to the newly created grid in one of the following ways:

  ▫ AGGREGATIONFILE followed by a DIDO aggregation file name.
    The DIDO file maps the reference grid towards this new grid. Because DIDO works on the hydrodynamic grid, the reference grid in this case will almost always be the *base grid*. Since DIDO only works on one layer, it will only contain the aggregation of one layer.
  ▫ as many integers as the reference grid has computational cells, each indicating the cell number of the newly created grid that is containing the corresponding cell of the reference grid.

In our mentioned example the grid definition section defines the:

◇ water-grid
  using an include file that just contains the numbers 1 to 1430 and is thus an exact copy of the grid in the water phase.
◇ water-zone
  using 1430 times the number 1. So this grid has only 1 grid cell that contains all of the computational volumes of the water phase.
◇ sediment-grid
  also using 1430 numbers. The mentioning of the reference grid is superfluous because it is the *base grid* that is also the default reference grid. The 1430 numbers are mostly zero (for the water phase) and 110 of them have sequence numbers for the sediment columns that will be located underneath the corresponding water cell.
◇ sediment-zone
  This grid refers to the just created sediment-grid and thus has 110 entries in our example. The first 25 are all 1, the next 60 are all 2 and the last 25 are all 3. This indicates that this grid has 3 cells, containing all cells with a sediment column. This grid has made a zonation of the sediment collumns into 3 zones.
◇ sediment-default
  This grid refers to the just created sediment-zone and thus contains 3 entries, all being 1. So this grid has only 1 cell.

We have defined 3 BOTTOMGRID grids. That is a bit much since there is only one real *bottom grid*. The D-Water Quality input processor assumes that the first time a BOTTOMGRID is defined, that this grid should be considered as **the** *bottom grid*. It also tells so in output

warning statements. In our example this is the `sediment-grid` with its 110 cells, so one bed-column underneath each water column.

3.4 NOBOTTOMLAY keyword

Now we have to specify the number of sediment layers in the bed. This is done in one of the following ways:

◇ the `DEFAULT` keyword
This keyword should be followed by an integer indicating the amount of sediment layers that will be distinguished. This amount of sediment layers will appear underneath the water at all of the locations of the *bottom grid*.

◇ the `INPUTGRID` keyword
This keyword should be followed by an existing grid name / ID.
Then a number of integer values should follow, equal to the number of grid cells in the selected input grid. Each value tells D-Water Quality that that sediment column of that grid cell has as many layers as that integer amounts. In our example we mentioned the `sediment-zone` grid as the input grid. In this way the cells from the *bottom grid* have been grouped in zones, that each have an equal number of sediment layers. In our example the zone 1 has 10 sediment layers, zone 2 has 8 sediment layers and zone 3 has 5 sediment layers. What D-Water Quality will do is the following:

- ◻ All cells of the `INPUTGRID` (3 on our case) get their value (10, 8 and 5 in our case)
- ◻ Because the input grid is not the *bottom grid* (that is the `sediment-grid` in our case), the grid that is used as reference grid of the `INPUTGRID` get their values (all 110 in our case) based on the mapping process of the input grid on to the reference grid of that grid.
- ◻ This procedure continues until **the** *bottom grid* is reached and then the procedure stops. So this allows also for nested zonations, that could be useful for different reasons.

This construction allows an easy way to:

- ◻ define the number of layers in the sediment columns for the *bottom grid*:
  use the *bottom grid* as `INPUTGRID`
- ◻ define the number of layers per zone of the *bottom grid*:
  use the `sediment-zone` grid as `INPUTGRID`
- ◻ define the number of layers equal for the whole area:
  use the `sediment-default` grid as `INPUTGRID`, or directly use the `DEFAULT` keyword.

◇ the `ALL` keyword
This directly reads all values for the *bottom grid*, so it is equivalent with using the *bottom grid* as `INPUTGRID`

Note: that it is easy to create the sediment zonation using the DIDO-ASCII aggregation files with a graphical user interface. Once the zonation has been done, you can easily specify for each zone a separate value by using the zoned grid as input grid. We will meet that construction also later on in the input file where process constants and other process variables and where initial conditions have to be set, depending on a certain zonation of the model area.

3.5 BOTTOMGRID_FROM_ATTRIBUTES keyword

This keyword is used to indicate that the bottom grid is to be constructed directly from the attributes for each water segment. These attributes are normally specified in a so-called attributes file (extension: <atr>) and can be used to identify which segments are just above the bottom of the water body. The keyword was introduced to solve a problem with models where "z-layers" are used: the number of water segments will vary per column.

If this keyword is used, the next information should be in the form of an attributes file. So, typical use is:

```
BOTTOMGRID 'bottom'
REFERENCEGRID 'Base grid'
BOTTOMGRID_FROM_ATTRIBUTES
INCLUDE 'generated-file.atr'  ; attributes file as generated by the hydrodynamic model
```

3.6 SUBSTANCE_PROCESSGRID keyword

This keyword has to do with the *process decomposition* features in D-Water Quality. It is possible to compute a subset of the substances on a coarser grid than on the *base grid* of the D-Water Quality simulation. This option will

◇ transport the selected substances on the finer *base grid*
◇ at the time the processes should work those substances are averaged to the coarser grid
◇ the processes will be conducted on the coarser grid
◇ the resulting mass on the coarser grid will be subdivided over the finer *base grid* using their proportional weighting before the process step
◇ next transport step(s) will be set on the finer grid

This option is especially valuable if the water quality kinetics are expensive to compute and if they can be grouped into model zones that more-or-less behave identical with respect to the water quality processes. The aggregation and disaggregation steps are fully mass conserving, so the whole procedure remains fully mass conserving and the substances remain transported on the finer *base grid*.
The procedure is triggered by the SUBSTANCE_PROCESSGRID keyword. Then one of the following options should come:

◇ the ALL keyword
   This indicates that all substances will get their processes evaluated on the grid that will be selected.
◇ a list of substance IDs
   This will select the indicated substances to operate on the grid that will be selected.

Finally the ID of an already earlier defined grid should follow. This will make the selected substances to get their process kinetics on the coarseness of the selected grid. Again, it is easy to create a zonation of the grid for this aim, using the Graphical User Interface and the DIDO tool.

3.7 PROCESS_TIMESTEP_MULTIPLIER keyword

This keyword has to do with the *process decomposition* features in D-Water Quality. It is possible to compute a subset of the substances with coarser time steps than the selected transport time steps of the D-Water Quality simulation. This option will

◇ transport the selected substances on the finer *transport timer*

◇ at the time the processes on the substances should work, they are invoked
◇ next transport steps will be set on the finer transport time scale and so on.

This option is especially valuable if the water quality kinetics are expensive to compute and if they can be grouped to joint coarser time steps. There is also a reverse reason for using this procedure. It can be required to model the transport of substances with a relatively fine time step of say 10 seconds to preserve accuracy of spatial transport patterns. Water quality processes can however easily be evaluated every half hour. This option does that job.

◇ The procedure is triggered by the `PROCESS_TIMESTEP_MULTIPLIER` keyword.
◇ Then one out of the following two options should come:

  □ the `ALL` keyword
    This indicates that all substances will get their processes evaluated on the coarser time step.
  □ a list of substance IDs
    This will select the indicated substances to operate on the coarser time step.

◇ Finally an integer should follow that specifies the selected multiplier on the transport time step for the selected

D-Water Quality automatically sets the time step of the processes that act on the mentioned substances to the required time step for the substances. The default multiplier for the not mentioned substances is 1. This may lead to inconsistencies if the process acts between two substances that have different time step multiplier. These inconsistencies have been dealt with for the two most commonly applied sets of substances on different time scales, the `BLOOM` module for algae species competition and the `CHARON` module for equilibrium chemistry minimizing Gibbs free energy. Their time step size will overwrite any specified time step mutiplier of this section. It is generally safe to choose for all modelled substances a time step multiplier that is the same, e.g. 30 if you would want to model water quality with time steps of half an hour and transport of substances with 1 minute. A common time step size for the `BLOOM` algae competition process is 1 day.

3.8 Printed grid layout

It is often useful for models on a detail schematization, to inspect the behavior in certain areas in more detail. D-Water Quality allows you to specify a lay-out of grid numbers. If you do so, concentration and other output are produced in an ASCII output file exactly in the order of appearance in the specified grid layout. D-Water Quality uses the monitoring timer to produce this output. You may inspect gradients by specifying a printed grid output for a number of nearby computational volumes. If you see artifacts in the model output, you can analyze the likely reason for them to appear.

Where is which computational volume located? That can be inspected in 2 ways. One is using the DIDO tool. It shows the horizontal grid and allows you to inspect cell indices and cell numbers. Another one is using one of the standard graphical post-processing options and plot the grid only. You are then able by point and click to see grid cell numbers and indices at certain locations.

Specification of a printed grid layout starts with telling D-Water Quality where the grid comes from by one of the following:

◇ The keyword `NONE`, indicating that no printed grid will be used.
◇ The integer '-1' followed by an `ASCII` file name indicating where the description can be found. This option is the outdated equivalent of the present `INCLUDE` option.
◇ The integer '0' followed by a file name of a binary file that will contain the layout of grid cells.

◇ The integer '1' indication that information will follow in this file.
◇ The integer '2' that is the outdated equivalent of the `NONE` keyword.

For the options '-1', '0' and '1' two integers should follow:

◇ nx
An integer specifying the horizontal amount of grid cells to be printed. If a zero is specified, the printed grid layout will NOT be used. If a positive integer is specified, lines with that many values (of 15 positions each) will be produced in the output file.
◇ ny
An integer specifying the vertical amount of grid cells to be printed. If nx was non zero and ny is zero, then printed output is NOT used.

For options '-1' and '1' the following follows in the `ASCII` file, for option '0' in the binary file.

◇ ny lines with nx integers
The integers refer to the sequence numbers of the computational volumes. A zero indicates that a blank field should appear at that location in the printed grid. The same segment number may appear multiple times in the matrix.

```
                 1        ;      grid layout in this file
                 8        6      ;   the nx and ny values
     212  213  214     0     0     0     0     0      ; the grid
     306  307  308     0     0     0     0   313
     400  401    0     0     0   405   406   407
     494  495  496   497   498   499   500   501
     588  589  590   591   592   593   594   595
     682  683  684   685   686   687   688   689
```

is a valid specification of a printed grid layout.

3.9   Properties or attributes of computational volumes

For D-Water Quality each computational volume is equal. They are connected with each other through their joint interfaces and feature transport from one volume to the other through those interfaces. For the water quality processes some computational volumes are more equal than others. Some may be located at the water surface in a 3-dimensional model set-up and thus have reaeration of oxygen and CO_2 at the water surface. Others may be located at the bed and may have sediments underneath, with associated sediment processes. These are generally fixed properties, although the property "*has a water surface*" may change during the simulation with the water level in models with fixed Z-layer depths. Besides the fixed properties there may also time variable properties be specified through the D-Water Quality input processor. This however is seldom done and if done it is probably most useful to let them be created by a hydrodynamic model as e.g. in the case of drying and flooding in a model featuring tidal flats.

This section describes the specification of the currently implemented properties in D-Water Quality. It is possible to specify additional properties in the same way and to use them in your own process routines. There is however a *caution*: in later versions of D-Water Quality we may use the property number that you also are using. In that case you would not be able to follow our upgrades. You can minimize that risk by using property numbers that have a higher index number than the current maximum, because we tend to number them sequentially. Furthermore standard D-Water Quality property numbers are likely to come with a frequency of 1 per decade, so the risks are not high. The properties are stored as decimal entries in a 32 bits integer. That means that the current maximum of properties is 9 and that the range of

property values for all properties is from 0 to 9. The presently implemented 4 properties are given in table 3.2.

Table 3.2: Properties of D-Water Quality computational volumes

number	values	property
1	0	Volume is not part of the model (dry, land etc.)
	1	Volume is part of the active grid
2	0	Volume is both at top and at bottom of the water column. This holds for all volumes of a depth averaged model.
	1	Volume is at top of the water column
	2	Volume is neither at top nor at bottom of the water column
	3	Volume is at the bottom of the water column
3	?	Unknown functionality associated with GEM
4	n	Ownership table used for parallel computing

If the first attribute is not set, then D-Water Quality sets it at the default value of 1 for the whole model area. If the second attribute is not set, then D-Water Quality sets it to 0 (depth averaged cells) for the whole model area.

3.9.1 Constant attributes

The following input structure applies:

⋄ number of blocks of input
If zero, no further input is accepted for constant attributes.
⋄ that many sets of:

☐ number of properties in this block
☐ the property numbers of these attributes
☐ one out of 3 possibilities:

○ the BINARY_FILE keyword and a sting with the file name.
This option expects a binary file with for each computational volume an integer indicating the property(s) for this grid cell.
○ the DEFAULTS keyword

▷ the default property value that will be used for all cells
▷ the number of overridings
▷ that many pairs of a segment number and the property value to be used for that segment / volume

○ the direct specification of all properties of the computational volumes in the order of their segment number.

At the moment only the properties 1 and 2 are generally provided through the input file. So the choice is providing them separately or providing only one of them on the one hand or providing them jointly on the other hand. Joint properties may look like:

◇ 00 for inactive cells outside of the computation
◇ 01 for active cells in a depth averaged model
◇ 11 for cells at the water surface of a 3D model
◇ 31 for cells at the bed of a 3D model
◇ 21 for cells somewhere between the bed and the water surface

In general the hydrodynamic models with a supported interface with D-Water Quality all produce the required property information in a file that can just be included in D-Water Quality input processing without further adjustments by the user. The user may edit this file if the water quality processes in almost dry cells require that these cells are manually excluded from the computation. Then changing of the property of those cells to zero will do to xclude the cells.

3.9.2 Time variable attributes

The following input structure applies:

◇ the number of time variable properties.
   If zero, no further input is accepted for time variable attributes.
◇ the property numbers of these attributes
◇ the name of a binary file that contains these properties as a time series.

3.10 Segment volumes

D-Water Quality needs a mass conserving hydrodynamic set of volumes and flows. These form the coefficients in the advection equation. The diffusions, the interface areas and the characteristic distances between the volumes form a second set of coefficients, they complete the input for the advection - diffusion equation. It could be well argued to locate all of this input into one input group. That is done, they are in input group 4. For historical reasons there is however one exception and that are the volume values of the segments / computational cells. They are contained in this group 3. Volumes distinguish themselves from other hydrodynamic input in a number of ways:

◇ There are as many volume values as there are volumes. This number is called `NOSEG` and is equal to the amount of active cells in the *base grid*. The other hydrodynamic input has as dimension the number of exchange surfaces between volumes. This dimension is called `NOQ`. For 1-dimensional models `NOQ` is generally of the same order (but generally not equal to) `NOSEG`. In 2 dimensional models `NOQ` is generally about 2 times `NOSEG` and in 3-dimensional models about 3 times `NOSEG`.
◇ The volumes are given at certain times. They give the exact volumetric value at that time. All other hydrodynamic input describe the average value of the coefficients during the time step. By convention the *time stamp* of the records of the other coefficients is the start time of the time step of their functioning, that runs from that value to the time stamp of the next record.
◇ D-Water Quality can compute with time steps that are smaller than the time steps in the hydrodynamic files. Those time steps are then subdivided. To ensure mass conservation the volumes in between two *time stamps* are interpolated. Because the other hydrodynamic information is assumed to count for the whole time step, they are not interpolated but taken constant during the hydrodynamic time step. This procedure is furthermore called a *block function* contrary to the *linear interpolated* volume function.

The volumes are read through the standard input procedure for hydrodynamic data that is described in the Annexes. Per computational volume (or segment) one value is read. One scale value applies. As seen from the sample input file at the start of this chapter, this part of

the input is most commonly limited to '-2' and the name of the volumes file that was generated by the hydrodynamic model. Also input of '-4' and the name of a `MULTIPLE_HYD` file is regularly used. Be aware that the amount of values that is expected per time step is exactly equal to `NOSEG`, the number of active cells in the *base grid*. The value of the *time token* of each record in the time varying setting should be consistent with the integration timers and output timers.

3.11 Finalization

This part of the input file is finalized with the `#3` end of third data group indicator.

4   Hydrodynamic data

This is the fourth group in the input file. This group may read like:

```
;     fourth block of model input (transport)
  112000  ; number of exchanges in direction 1 (NOQ1)
  112000  ; number of exchanges in direction 2 (NOQ2)
  109200  ; number of exchanges in direction 3 (NOQ3)

  0  ; number of additional dispersion arrays
  0  ; number of additional velocity arrays

  1  ; first form of the input file structure is used

  0  ; exchange pointers come from a binary file
 'com-Bodensee.poi'   ; pointers file

  1  ; dispersions follow in this file
  1.0    1.0    1.0  ; scale factors in 3 directions
1.0e+00 1.0e+00          ; dispersion in 1st and 2nd direction
            1.0e-07  ; dispersion in 3rd direction

 -2  ; areas will be interpolated from a binary file
 'com-Bodensee.are'   ; area file

 -2  ; flows will be interpolated from a binary file
 'com-Bodensee.flo'   ; flow file

  1  ; spatially varying exchange lengths
  0  ; lengths come from a binary file
 'com-Bodensee.len'   ; length file

#4 ; delimiter for the fourth group of input data
```

4.1   General

Group 3 of the input file already contained information that is associated with the schematization of the model and the water flow. It contained the number of computational volumes / cells / segments (names that are all equivalent). It also contained a description of the input of the (time series) of the volumes in m^3 for each of these segments. Group 3 also contained information on the properties of these cells / segments (dry or wet, at the top, at the water bed or in the middle).

In group 4 of the input file this information on model schematization and hydrodynamic information is continued with flows across the exchanges and other transport related information. Most of the time, hydrodynamic input will be substantial and will be generated by hydrodynamic models. For these situations the input as given in the example at the start of this chapter is typical and it is also the minimal input required. We will run through this example input here to explain the different input items. There are much more additional options per input item than mentioned in this explanation and they are discussed in detail in the sections that follow in this chapter.

◇ The number of exchanges in each direction

  ▢ This 'Bodensee' model typically is a model on a structured curvilinear mesh, because it has exchange interfaces in three directions. This means that 2 separate horizontal directions exist. Models with unstructured grid generally have only one total number of exchanges for direction 1 and zero for the number of exchanges in direction 2.
  ▢ It is a 3-dimensional model. Depth averaged models have zero for the number of exchanges in the third direction.

- ▫ The model is apparently using a grid that consists of a full matrix (with many zero's at locations in the matrix with dry entries). This can be inferred from the exactly equal number of exchanges in both horizontal directions. For models on matrices of grid cells with only the active cells and active exchanges mentioned, the number of active exchange surfaces in the two horizontal directions is generally not exactly equal.
- ▫ One layer of the model apparently has 2800 grid cells. This is the difference between the number of exchanges in one horizontal direction and in the vertical direction. There is one layer of exchanges less in the vertical, because between n layers there are only n - 1 interfaces.
- ▫ It is a 40 layer model because the number of horizontal exchanges in one direction divided by 2800 is exactly 40.

D-Water Quality also makes these inferences, but it also allows for the direct specification of the number of layers and it does not require full matrices of input, it even does not require a structured grid.

◇ The number of additional dispersion arrays
D-Water Quality has constant dispersion coefficients (diffusion coefficients that account for the turbulent diffusion and the additional mixing at coarser grids additional to molecular diffusion) in the three mentioned exchange directions. You can furthermore specify additional spatially varying dispersion coefficients per exchange surface. You do so by specifying a non-zero the number of additional dispersion arrays here. You might think that you need to do so if you want to use the vertical diffusions that are generated by the turbulence model of the hydrodynamic model. That however is not the case. The hydrodynamic model will produce the vertical diffusions per cell and not per exchange. In group 7 of the input file you will specify the vertical diffusion file that is produced by the hydrodynamic model. There also the 'process' will be switched 'on' that creates an additional diffusion array and puts the vertical coefficients therein. You just specify zero here.

◇ The number of additional velocity arrays
For additional velocity arrays the same holds, but now the information on the magnitude of the additional velocities is most often generated by the processes library itself as e.g. settling velocity of particles. Also in that case just state zero here, because the processes library will itself automatically make the necessary additional velocity arrays and put the settling velocities in the section of the third dimension, the vertical.

◇ form of the input file structure
The first form of input is used here. The second form is documented in a following section. It is rarely used because it is mainly convenient for the manual specification of the hydrodynamics of relatively small models.

◇ exchange pointers
The number of exchanges was specified earlier. Now for all of these exchanges it should be specified between which cell numbers the exchange surface is located. That happens with this part of the input.

◇ dispersions
These are the constant dispersions that will act on all transported substances and will be added to the dispersion array values. If additional dispersion arrays were specified, they should be given values here. In the example this part can be absent.

◇ velocities
If additional velocity arrays were specified, they should be given values here. In the example this part can be absent.

◇ areas
These are the exchange surface area magnitudes in m^2 that are used to compute the diffusive exchange flux in m^3/s with: $flux = \frac{D \cdot A}{length}$.

◇ flows
These are the flows across the exchange surfaces in m^3/s

◇ lengths

These are the exchanges lengths in the diffusive flux formula. They can be spatially constant for a rectilinear grid, but it is most common that they are spatially variable. In all cases it is most common that the file of values is generated by the hydrodynamic model like in this example.

In the following sections all topics are discussed in more detail.

It should be mentioned again that the examples of the input generally are given in a nicely formatted way. The positioning of the data on the input lines is however irrelevant. Only the order of the input matters and input items should be separated by at least one blank. The same model result as with the example at the start of the chapter would be obtained with e.g.:

```
112000 112000 109200 0 0 1 0 com-Bodensee.poi 1 1. 1. 1. 1. 1. 1.e-7
-2 com-Bodensee.are -2 com-Bodensee.flo 1 0 com-Bodensee.len #4
```

4.2 Number of exchanges

4.2.1 Standard processing for irregular solvers

D-Water Quality requires three integers here:

◇ The number of exchanges in the first horizontal direction: NOQ1.
◇ The number of exchanges in the second horizontal direction: NOQ2 or zero if it does not exist.
◇ The number of exchanges in the third, vertical direction: NOQ3 or zero if it does not exist.

4.2.2 Processing for solvers on regular grids

Solvers 19 and 20 use a technique call ADI - Alternate Direction Implicit. They stem from the regular grid Delft3D-FLOW environment and use almost identical source code. These solvers require a matrix topology of grid cells. The dimension of this matrix is read from the input file at this location. Also 3 integers are required, but they have different meaning:

◇ the size of the fastest running (first) horizontal index of the matrix topology, called NMAX.
◇ the size of the slowest running (second) horizontal index of the matrix topology, called MMAX.
◇ the size of the third index in the matrix topology, called KMAX.

Unlike the input for irregular solvers, you now must specify 1 for the 3rd direction if the model is depth averaged, since then there is one layer of computational cells in the matrix. For a size of zero the matrix would disappear.

4.3 Number of additional dispersion and velocity arrays

Both for additional dispersions and velocities the following input structure holds:

◇ integer number of additional dispersion / velocity arrays
◇ for each of these arrays a string of at most 20 characters giving the ID of the array
◇ for each modeled *transported* substance (so not the passive substances) an integer that indicates which array should be applied for that substance. Zero is required if no additional array should apply to the substance.

like:

```
1     ; number of additional dispersion arrays
```

```
'random swimming fish'
0  0  0  0  0  0  1  1  1  0  0      ; for the 11 transported substances
2    ; settling velocities of particulates
'v-s inorg. partic.'
'v-s org. partic.'
0  0  0  1  2  2  0  0  0  0  0      ; for the 11 transported substances
```

4.4 Exchange pointers

The specification of the grid cell /segment numbers at both sides of an exchange surface is done by the specification of four integers for each exchange surface:

1 the number of the 'from' segment
2 the number of the 'to' segment
3 the number of the 'from-1' segment
4 the number of the 'to+1'segment

The following properties can be identified:

◇ the selection of the 'from' and 'to' segment numbers also defines the positive direction of flow through the surface. Negative flow runs from 'to' to 'from'.
◇ for an open boundary cell / segment one specifies $-n$ with n the sequence number of that open boundary.
◇ for closed boundaries and connecting inactive cells you may specify zero or you may alternatively omit the specification (and then also state that you have a lower number of exchanges in that direction of course).
◇ the 'from-1' and 'to+1' entries are only used for some higher order scheme's (5, 12 and 14). If you do not use that solvers then you can just specify zero for these two entries.
◇ D-Water Quality will just skip the entry in the computation if one of the 'from' or 'to' numbers is zero or if both are zero and/or negative. Also the flow, area and lengths that are found at that location in the files are neglected.

The table of 4 integers per exchange surface can be specified to D-Water Quality in several forms. You start with an integer option number:

0 input comes from an external binary file
Optionally now `UNFORMATTED` and `BIG_ENDIAN` may be used as keywords to indicate that the file structure deviates from the default of `BINARY` and `LITTLE_ENDIAN`. Then the name of the file follows. This is generally the way to couple D-Water Quality with the administration of a hydrodynamic model. The file contains:

◇ For most solvers:
`NOQ1` + `NOQ2` + `NOQ3` groups of 4 integers. The implementation for `UNFORMATTED` files is such that each group of 4 integers forms a record.
◇ For solvers on regular grids (e.g. 19 and 20):

□ Seven integers (in one record for `UNFORMATTED` files): `NMAX`, `MMAX`, `NOSEGL`, `KMAX`, `NOQ1`, `NOQ2`, `NOQ3`. These seven integers are checked against earlier input to identify that the file contents is compatible. `NMAX`, `MMAX`, `KMAX` should correspond. `NOSEGL` is the highest active grid cell number that will appea in the matrix and `NOQ1`, `NOQ2`, `NOQ3` are the number of areas and flows that will be contained in the corresponding hydrodynamic files.
□ The complete matrix of segment numbers (or zero for inactive grid cells) of one layer. It has the size of `NMAX`*`MMAX` and is in one record for `UNFORMATTED` files.

1 input comes from this `ASCII` input file

Optionally you may use the `INCLUDE` directive like everywhere in the D-Water Quality input file. The input now contains:

◇ For most solvers:

`NOQ1` + `NOQ2` + `NOQ3` groups of 4 integers, like for Venice Lagoon at unstructured grid:

```
   1    2    0    0
   1    3    0    0
   2    3    0    0
  ..   ..   ..   ..
2228  2256   0    0
2228  2255   0    0
  -9  2230   0    0
   0     0   0    0
2230   -10   0    0
2231  2232   0    0
```

◇ For solvers on regular grids (e.g. 19 and 20):

□ Four integers: `NMAX`, `MMAX`, `NOSEGL`, `KMAX`. These four integers are checked against earlier input to identify that the file contents is compatible. `NMAX`, `MMAX`, `KMAX` should correspond. `NOSEGL` is the highest active grid cell number that will appear in the matrix.

□ The complete matrix of segment numbers (or zero for inactive grid cells) of one layer. It has the size of `NMAX*MMAX`.

4.5 Dispersions

4.5.1 Dispersion input through the input file

The input of dispersion coefficients as conducted by the general procedure for hydrodynamic input data that is described in the Annexes. It should be noted that if no additional dispersion arrays are specified, then only the constant dispersion coefficients need to be read (like in the example input at the start of the chapter). Further dispersion coefficients may be read here if the specified number of additional dispersion arrays is non-zero.

◇ If the first option number for the reading of the dispersion information is not zero, then the constant dispersion coefficients per direction in the grid will be added to the specified dispersion coefficients.

◇ If the first option number for the reading of the dispersion information is zero, then the constant dispersion coefficients per direction in the grid are not read and get a default value of zero.

4.5.2 Dispersion input through the processes library

4.5.2.1 The VertDisp process

You will have seen that the standard input as provided at the start of this chapter looks much more simple than the above specification. No additional dispersion arrays are specified and yet only the constant values needed to be specified per direction. Is it then common that D-Water Quality only uses constant dispersion values in space and time? How about stratification? No, it is only common that D-Water Quality uses constant horizontal dispersions, but that D-Water Quality uses the outcome of the hydrodynamic turbulence model for the vertical dispersions. This vertical dispersion is generally specified as a segment function (see group 7 of the input file) with the name `VertDisper`. This segment function is input for the process `VertDisp` that is also switched 'on' in that group of the input data. The process will automatically create an additional dispersion array and will switch it 'on' automatically for all

substances that are transported by water. The additional dispersion array has values zero in the horizontal directions and has the vertical diffusion coefficient that was generated by the hydrodynamic turbulence model. The constant horizontal and vertical diffusion values specified in this input file are added to the values that are generated by the processes library. So in our sample case the horizontal diffusion coefficients will be 1.0 m^2/s and the vertical diffusion coefficients will be 1.0E-07 + the value from the hydrodynamic model in m^2/s. There is an input item for the process `VertDisp` called `ScaleVdisp` with default value 1.0 that allows for scaling of the vertical diffusion as generated by the hydrodynamic model.

We are at the advent that hydrodynamic models may produce spatially varying horizontal dispersion coefficients using `HLES` (Horizontal Large Eddy Simulation) models. This development is induced by the use of increasingly smaller horizontal grid cells. The smaller the horizontal grid cells are, the more important the local differences in horizontal mixing coefficients will be. Once models deliver such files for the horizontal direction with included vertical coefficients in the vertical direction, the use of the '-4' and '-2' option of the preceding section together with the declaration of an additional dispersion array, will do to incorporate such developments in D-Water Quality.

4.5.2.2 The VertDisper process

If the hydrodynamic model does not produce a file with the vertical diffusion coefficient as computed by a turbulence model, then there is an alternative. You can model salinity and temperature, let the water density be computed and switch 'on' the process `VertDisper`. It uses the common formulae that relate density gradients and gradients in the horizontal velocity to vertical diffusion coefficients and also produces the Richardson number thus obtained.

4.5.2.3 The HDisperVel process

This process is generally used for depth averaged models. The horizontal dispersion coefficient should then have a strong, water flow direction dependent, component associated with the vertical shear in horizontal velocities that are neglected due to the vertical mixing. This process tries to substitute for this and create a horizontal mixing coefficient that is depending on the horizontal water velocity locally. It is however a very rude and inadequate solution since it is almost impossible to specify horizontal diffusion coefficients that run mainly along directions of about $45°$ with the grid lines, because decomposition in both directions then give equal dispersion coefficients in both directions. If horizontal dispersion is important, you are strongly advised to use a 3-dimensional model with at least 3 to 4 water layers. If you do so you can specify zero for the horizontal diffusion coefficient because the horizontal dispersion process is fully modeled by the shear in velocities.

4.6 The exchange areas between computational cells

The exchange areas between computational cells are used to:

1. Compute the diffusive mixing flux
   The diffusive mixing flux is computed from the dispersion coefficient D, the surface area A of the exchange surface between two cells, the distance between the cell midpoints at both sides of the exchange are and the difference in concentrations at both sides by: $Flux = -\frac{D \cdot A}{length}\Delta C$. The flux counteracts the gradient and is often seen as a diffusive flow of: $Dflow = \frac{D \cdot A}{length}$ in both directions, times the outgoing concentrations. A step even further is to attach a physical meaning to the $length$ term by calling it a *mixing length* which is of course erroneous since it is just the distance between the midpoints of the two adjacent cells and forms part of the concentration gradient: $gradient = \frac{\Delta C}{length}$.

2. Compute velocities
   D-Water Quality can model the complete advection diffusion equation without knowing the

water velocities. That is because it is a Finite Volume (FV) model. It solves the volumetrically integrated advection diffusion equations and uses flows rather than velocities for that. However for a number of water quality processes it may be necessary to know the water velocity. D-Water Quality computes this in the processes library by dividing the flow by the area where the flow goes through. To get the velocities in the cell midpoints (or the velocities that are representative for the cell as a whole) several averaging methods exist in the processes library to average values at the cell interfaces. Increasingly more however hydrodynamic model using unstructured grids are used. Then the averaging process is not so trivial any more. These models generally produce velocity files that are read by input group 7 of the input processor.

3 Compute the thickness of cells
   D-Water Quality compute the thickness of cells by dividing the volume of the cell by the horizontal surface area of the cell. This gives a time varying thickness value that is used in processes that e.g. compute the extinction of visible light in the vertical etc.

4 Compute superficial processes
   D-Water Quality uses the horizontal surface area of cells to e.g. compute reaeration of oxygen at the water surface or to compute the amount of settled sediments per m^2 of the bed.

The exchange areas for aim 1 and 2 are read in this section of the input file. The horizontal areas are also contained in this dataset if the model is 3-dimensional. If however the model is 2-dimensional depth averaged, then there are no horizontal exchange areas because there are no vertical fluxes and transports. That is why horizontal areas for aim 3 and 4 are separately stored in a variable called `SURF`. This variable is generally read as parameter or segment function in group 7 of the input file.

The exchange areas are read through the standard input procedure for hydrodynamic data that is described in the Annexes. Per exchange surface one value is read. One scale value applies. As seen from the sample input file at the start of this chapter, this part of the input is most commonly limited to '-2' and the name of the areas file that was generated by the hydrodynamic model. Also input of '-4' and the name of a `MULTIPLE_HYD` file is regularly used.

4.7 The flows between computational cells

The flows are essential for D-Water Quality in the solution process of the advection diffusion equation, but are also used in processes of the processes library. The input of flows is fully identical to the input of areas that is explained in the previous section. It also uses the standard input processing that is described in the Annexes and will not be described here. Also for this entry the '-2' and '-4' options are the most common options.

4.8 Velocities

If additional velocity arrays have been specified before, this is the place to specify there value, or where they will come from. Additional velocities are incorporated in the solution of the advection diffusion equation like the additional dispersions are. They act on the substances where they have been specified for. If '0' was specified as additional velocity array number for a substance then no additional velocity is applicable. Additional velocities generally play a role as settling velocities and floating velocities of particulate substances heavier than water or lighter than water. These velocities are generally computed by the processes library by transport processesand automatically stored in arrays and applied for the substances where they are ment for. So generally you then specify zero additional velocity arrays and this section of the input file can be fully omitted.

Should you want to add additional velocity arrays yourself, then you follow exactly the same

input procedure as for areas and flows. The only difference is that if you specify 4 additional velocity arrays, then you should apply the procedure for 4 values per exchange rather than for one value per exchange as done for areas and flows. There is still 1 scale value per direction `NOQ1`, `NOQ2` or `NOQ3` when present.

4.9 Lengths

The lengths between the midpoints of computational cells at both sides of interface areas are used to:

1 Compute the diffusive mixing flux
   The diffusive mixing flux is computed from the dispersion coefficient D, the surface area A of the exchange surface between two cells, the distance between the cell midpoints at both sides of the exchange are and the difference in concentrations at both sides by: $Flux = -\frac{D \cdot A}{length}\Delta C$. The flux counteracts the gradient and is often seen as a diffusive flow of: $Dflow = \frac{D \cdot A}{length}$ in both directions, times the outgoing concentrations. A step even further is to attach a physical meaning to the $length$ term by calling it a *mixing length* which is of course erroneous since it is just the distance between the midpoints of the two adjacent cells and forms part of the concentration gradient: $gradient = \frac{\Delta C}{length}$.

2 Weigh concentrations in central schemes
   If two adjacent cells differ strongly in size, one may distinguish the distance of the 'from' cell midpoint to the interface area and of the 'to' cell midpoint to the interface area. This intuitive separation of two distances is also implemented in a number of higher order 'central' numerical schemes. This approach is increasingly more considered mathematically questionable and is easily eliminated by the specification of two equal half values of the total distance between the cell midpoints rather than the two half values of the unequal cell sizes. The latter have the same sum, but differ from each other.

Horizontal distances between cell midpoints are generally constant over time. This may produce a relatively small file with one specification that will hold for the whole simulation period. In 3-dimensional models the water level change will change the vertical distances though. To avoid huge files for this item, you can just specify vertical lengths of zero for this specification. D-Water Quality will automatically fill in the correct vertical distances from the thickness of cells as computed per time step by the cell volumes divided by the horizontal surface areas. There are two options to specify lengths to D-Water Quality

0 Lengths are constant spatially and in time
   This requires 1 scale value and 3 lengths values for the 3 dimensions. So in this case no half lengths are specified and the third value is also required for depth averaged 2-dimensionlan models. This option would only be appropriate for a sort of test cube of identical small cubes as computational volumes.

1 Lengths vary spatially
   This requires exactly the same input structure a for areas, flows and velocities with special consideration that 2 values are needed per interface area, the 'from'-length and the 'to'-length respectively. Per direction 1 scale values is required for `ASCII` input.

4.10 Second form of input file structure

This chapter up to now documented the first form of the structure of the input file. Once you have read the information on items that are contained in this input, you will also understand the meaning of the input items in this simple alternative second form of the input. It is a tabular input with:

◇ four scale factors for:

  □ dispersions
  □ areas
  □ flow
  □ lengthes

◇ NOQ1 + NOQ2 + NOQ3 rows with:

  □ 'from' cell number
  □ 'to' cell number
  □ 'from-1' cell number
  □ 'to+1' cell number
  □ dispersion in m^2/s
  □ exchange area in m^2
  □ flow in m^3/s
  □ 'from'-length in m
  □ 'to'-length in m

Like in:

```
        1       ;  information in this file
                    1.0   1.0   1.0     1.0   ; scale factors
;   from  to  fr-1 to+1   D    A     Q      L
    -21   65  -21  66     5 1500 1500  250   250
    -22   81  -22  82     5 1500 1500  250   250
     17   18  -18  19     5 1500 1500  250   250
     18   19   17  20     5 1500 1500  250   250
     19   20   18  21     5 1500 1500  250   250
     20   21   19  22     5 1500 1500  250   250
     21   22   20  23     5 1500 1500  250   250
     ..   ..   ..  ..    ..   ..   ..   ..    ..
```

4.11 Finalization

This part of the input file is finalized with the #4 end of fourth data group indicator.

5 Open boundary conditions

This is the fifth group in the input file. This group may read like:

```
  ;  Open boundaries
    'River      1'  'River Williamsburg side  '  'River'
    'River      2'  'River 100m from bank     '  'River'
       ....              ....                       ....
    'River     12'  'River Brookmarsh side    '  'River'
    'Ocean      1'  'Ocean at Cape Cod side   '  'Ocean'
       ....              ....                       ....
    'Ocean    100'  "Ocean at Mary's Lighthouse"  'Ocean'

           1          ; Thatcher-Harleman time lags for all entries
  ;       hhmmss
       12*10000       ; 1 hour for first 12 entries (River)
       100*3000       ; 30 min. for next 100 entries (Ocean)

   ITEM                           River   Ocean
   CONCENTRATION Salinity DATA    0.1     34.5

   ITEM                 'River'
                        'Ocean'
   CONCENTRATION  USEFOR  Continuity   Cont
                  USEFOR  Oxy          O2
                  USEFOR  PO4          Tot-P  -  Part-P  MIN  0.0
                  USEFOR  AAP          Part-P
  TIME  LINEAR  DATA  Cont  Tot-P Part-P NO3-N  O2
2012/01/01-12:00:00   1.0   0.15  0.1    1.7    7.5   ; river
                      1.0   0.05  0.03   0.5    8.4   ; sea
2012/02/01-12:00:00   1.0   0.10  0.07   1.0    8.0   ; river
                      1.0   0.05  0.03   0.5    8.4   ; sea
              ... ... ...
2013/01/01-12:00:00   1.0   0.15  0.1    1.5    8.5   ; river
                      1.0   0.05  0.03   0.5    8.4   ; sea

 #5              ; delimiter for the fifth group of input data
```

5.1 General

Open boundary conditions deal with the influence from outside of the model domain. To a certain extent also waste loads do. Open boundary conditions however distinguish in some important aspects from waste loads:

◇ Open boundary conditions are contained in the transport schematization that comes from the hydrodynamic model. They appear as negative integers in the 'from'-'to' pointer table for exchanges between the finite volumes. An entry of e.g. -6 refers to the 6th open boundary condition. Waste loads do not have entries in the 'from'-'to' pointer table.

◇ Open boundary conditions come with a flow from the hydrodynamic model. Waste loads may come with a flow from the hydrodynamic model, but may also be specified independent of the flow model. The latter generally happens for waste flows that are so small that they need not be contained in the hydrodynamic model. A city of 1 million inhabitants will e.g. generate a waste flow of about 1 m^3/s but that amount may be too small to influence hydrodynamic velocities in a tidal marine area.

◇ By default the numerical scheme is expanded across the open boundaries by having diffusion across open boundaries and/or having higher order flux correction terms across open boundaries. If you want these effects be switched 'off', you need to use the keywords NODISP-AT-BOUND and/or LOWER-ORDER-AT-BOUND in the group 2 section of the input file. If diffusion across open boundaries is used, e.g. for mimicking salt intrusion with a diffusion term for 1-Dimensional rivers entering a sea, the user must be aware

that the constant diffusion term of group 4 of the input file acts on all open boundaries. It is then best to set the constant diffusion to zero and to give nonzero values where needed to an additional diffusion array.

◇ It is possible to specify a 'Thatcher-Harleman' open boundary condition that will be discussed later in this section. For waste loads this option does not exist.

5.2 Identification of open boundaries

The input processor scans the 'from'-'to' pointer table for negative entries. These negative cell numbers refer to artificial 'open boundary cells' with that sequence number, at the outside of the model domain. The input processor reports the entry with the biggest sequence number that it found. It also indicates all those entries within the range from 1 to the highest entry that are not associated with an exchange surface with a model cell located within the model.

Because each exchange across the open boundary is an entry, the amount of entries can become quite large in 3-Dimensional models. To assist somewhat with the specification of open boundary conditions, there is the possibility to group the open boundaries with a 'type' indicator.

For each open boundary entry, also those that are not associated with a model cell, the following input is required:

◇ A boundary-ID. The first 20 characters of the boundary-ID should be unique.
◇ A boundary-name. This input is not used by D-Water Quality but assists the user in the identification of the open boundary entry. The first 40 characters are echoed to the listing file.
◇ A boundary-type. The first 20 characters of the boundary type are recognized and can be used to group the open boundary entries e.g. to the type 'Northern boundary'. For all entries of a type, one identical concentration can be specified.

It is possible to specify empty strings for all entries. If there are e.g. 112 open boundary entries, one could specify here:

```
336*" "
```

The net effect of this specification will be that D-Water Quality fills in:

```
'Boundary-ID      1'  'Boundary  name      1'  'Boundary type 1'
'Boundary-ID      2'  'Boundary  name      2'  'Boundary type 1'
   ....                    ....                    ....
'Boundary-ID    112'  'Boundary  name    112'  'Boundary type 1'
```

This is generally not so informative and also not so convenient. In the example at the start of the chapter we distinguished a 'River' boundary type and an 'Ocean' boundary type. This gives us opportunity to define a concentration at each of the two, without having to do so for all the open boundary cells individually. Should we, for a certain substance, want to have different values for the right bank and the left bank of the river and interpolate between them, then this is still possible using the 'River 1' to 'River 12' ID values for that substance alone. The names are not used by D-Water Quality but are helpful to identify which bank we are meaning. Note that we used in the example at the start of the chapter double-quotes around the last boundary name to enable the use of a single quote within the character string. The identification of open boundaries given here is also used in the output files with mass balance information to enhance the identification of the mass balance terms.

5.3 Thatcher-Harleman time lags

In general tidal open boundary conditions show an outflow during the out-flowing tidal half and an inflow during the inflowing tidal half. At the turn of the tide the first inflow will consist partly of the material that flew out in the hour before. To account for this you can specify a "Thatcher-Harleman time lag" for each open boundary entry. The time lag works as a half cosine function between the last outflow concentration at the time of last outflow (called t_{out} and the specified boundary concentration at t_{out} + the time lag, according to:

$$C_{in} = \begin{cases} \frac{(C_{out}+C_{bound})}{2} + \frac{(C_{out}-C_{bound})}{2} \cdot cos\left(\frac{t-t_{out}}{lag}\pi\right) & \text{if } 0 < t < t_{out} + lag \\ C_{bound} & \text{if } t > t_{out} + lag \end{cases}$$

For times since last outflow longer than the specified lag, the prescribed boundary concentration is applied. This means that the time lag feature is switched off by selecting 0 for the time lag.

You specify these time lags as integers. If you earlier specified to use DDHHMMSS format for times, then a time lag of 1 hour looks like 10000. If you did not specify that format, then you should enter 3600.

You have the following three input options, they start with a 'switch' integer that is 0, 1 or 2:

0 No time lags.
1 Time lags for all entries like in the example at the start of the chapter.
2 Time lags with a default value and specified exceptions:
  The exceptions consist of the entry number of the exception and the value to be used instead of the default value, like in:

```
        2           ; time lags with a default
;       mmss
        3000        ; default value of 30 min.
         12         ; number of exceptions....
;       hhmmss
    1   10000       ;   first exception
    2   10000       ;   second exception
      ........
   12   10000       ;   twelfth exception
```

Note: the exception number refers to the open boundary number. The fact that the 12th exception has number 12 is coincidental here.

5.4 Concentration values

If you specify furthermore nothing, then zero will be used as open boundary concentration for all substances and all boundary entries. Everything that you specify here will fill in just the entry that you specify. If you specify the same entry and the same substance twice, then the last specification will be used. If you first specify a high frequency sampled time series for an entry-substance combination and later on a lower frequency sampled time series for the same entry but for a combination of that entry with other substances, then both are applied. This means that you are fully flexible. The specification of concentrations is done through a number of input blocks, each containing the concentration values for a number of boundary entries and a number of substances.

5.4.1 Input blocks

The input is organized in blocks. Each block consists of the definition of the entries that are specified in the block, these are called ITEM. Furthermore the block definition consists of the substances that are specified in the block, they are called CONCENTRATION. The

`DATA` in a block consist of a (series of) matrices. If you first specified the `ITEM` entries, then the matrix consist of rows of concentration values. One for each item. If you first specified `CONCENTRATION` entries, then the matrix consists of rows per substance and values for the items on the rows. Be aware that D-Water Quality reads tokens only. D-Water Quality is not aware of the layout that you use for the input file. You may put all your information on one line, or you may put every item on a subsequent line. So you cannot leave a matrix entry blank and you cannot assume that a new row starts with a new line. A new row starts if enough data is read for the previous row. So if there is no value available, then you may specify -999.0 instead. This is interpreted by D-Water Quality as a missing entry.

Character strings may be embedded in single or double quotes. Quotes / double quotes are only required if there are embedded blanks or embedded quotes in the string.

So either:

```
ITEM
    'River outflow'
    'Northern boundary'
CONCENTRATION
    Salinity
    Continuity
    Oxygen
DATA  ; salinity  continuity   oxygen
        16.0        1.0        7.5        ;  river outflow
        35.0        1.0        8.4        ;  northern boundary
```

or:

```
CONCENTRATION
    Salinity
    Continuity
    Oxygen
ITEM
    'River outflow'
    'Northern boundary'
DATA  ;     river outflow      northern boundary
            16.0                35.0         ; salinity
            1.0                 1.0          ; continuity
            7.5                 8.4          ; oxygen
```

Note that 'River outflow' may be a boundary ID of a single entry, whereas 'Northern boundary' may be a boundary type consisting of many entries. Instead of a boundary ID, you may also give an integer value say 'i' as `ITEM`. D-Water Quality will then assume that you want to specify the boundary with sequence number 'i'. Furthermore there may be more open boundaries and substances in the model than those mentioned in this block. The others may be defined in subsequent other blocks. The strings behind the semi-colons are comment strings that are used here to make the table more readable.

5.4.2 Column headers and computations

Within one or more input blocks you may apply column headers that are no comments in the following way:

```
ITEM
    'River outflow'
    'Northern boundary'
CONCENTRATION
    USEFOR  Salinity     'Sal o/oo'
```

```
    USEFOR   Continuity     Cont
    USEFOR   Oxy            O2
    USEFOR   PO4            Tot-P  -  Part-P  MIN  0.0
    USEFOR   AAP            Part-P
 DATA
   'Sal o/oo' Cont Tot-P Part-P  NO3-N   O2
      16.0   1.0   0.15   0.1    1.7    7.5  ;  river outflow
      35.0   1.0   0.05   0.03   0.5    8.4  ;  northern boundary
```

Now the column headersare used as an identification of the column. They need not correspond with the reserved names of the processes library, but they can be linked through the `USEFOR` clause.

◇ Note that the order of the columns is not important.
◇ Note that the NO3-N column is not used.
◇ Note that computations are possible:

  □ The tokens and computational symbols should be separated by one or more blanks.
  □ `+`, `-`, `*`, `/`, MIN and MAX are possible as computational directives.
  □ They are evaluated in agreement with accepted math rules, i.e. `*` and `/` are evaluated before `-` and `+`. Brackets can not be used. If you want a*(b+c), then you should specify `a * b + a * c`.
  □ Instead of a column header token also a number can be used in the computations.
  □ The computations act on whole columns, so if your columns are items, then the computations may be less useful.

5.4.3 Time series

Up to now we have assigned one concentration value for each mentioned substance to each mentioned boundary item. It is however common to have time varying open boundary conditions consisting of a time series of concentrations. Time series start using the `TIME` keyword before the `DATA` keyword. This tells the input processor that this input block consists of a time series. Once you specified this keyword, D-Water Quality expects a series of matrices rather than a single matrix. The most simple time series consist of 2 matrices for 2 time stamps. Each matrix should be preceded by a 'time' indication. That can be:

◇ An integer in `DDHHMMSS` format if you specified to use that format in the group 1 input section.
◇ An integer in seconds if you did not specify to use the format.
◇ If you gave a reference time in the model ID strings in the group 1 input section, then you can also specify calendar dates here as e.g. `2012/02/28-12:35:00`. The two '/', the '-' and the two ':' characters are required exactly in this form, otherwise the time string will not be recognized.

D-Water Quality reads sets of a time and a matrix of data until it meets a reserved keyword (mostly `ITEM` or `CONCENTRATION`) that starts the subsequent data block. Also the `#5`, the end of block 5 signal, ends the processing of a time series.

5.4.4 Linear interpolation

The default processing of time series is that the specified value at a specified time is used up to the next specified time, a so-called block wave. Then the value switches to the next specified value. For one or more of the input blocks you may alternatively want to interpolate linearly in between two specified values at specified times. To make D-Water Quality interpolate your time series linearly, you insert LINEAR after the TIME keyword and before the DATA keyword. Also the BLOCK keyword is supported, but it is superfluous since this is the default processing of time series.

5.4.5 Scale your input

If you copy and paste large amounts of data into your input file, then it is cumbersome if the data does not have the units that are required for the simulation. If you have data in $mole$ or in $\mu g/l$ rather than the g/m^3 or mg/l that is required by D-Water Quality then it is convenient that you just scale your input. You do so by specifying the SCALE keyword before the DATA keyword. The SCALE keyword should be followed by as many scale factors as there are columns in the matrices that you will provide. So you must provide 1.0 for each column that will not be scaled. It is also possible to scale your input using the USEFOR clause and multiply there by the appropriate scale factor.

5.4.6 Data from external non-ASCII files

D-Water Quality supports the entry of data from non-ASCII self describing so called ODS_FILE files. This Deltares proprietary file format is not further documented here. The use of this option is to specify the ODS_FILE keyword followed by the name of the file. This specification is used instead of the DATA keyword and the data matrices that follow that keyword.

5.4.7 Multiple copies of substances

If the feature of multiple copies of substances is used, then for each copy a boundary condition must be provided. This is facilitated by the input structure through e.g.:

```
ITEM                'My Boundary'
CONCENTRATIONS
    USEFOR  IM101   IM1   * 0.25
    USEFOR  IM102   IM1   * 0.25
    USEFOR  IM103   IM1   * 0.50
TIME LINEAR
DATA                   IM1
1990/08/05-12:30:00   1.00e+001
1990/08/06-01:00:00   1.20e+001
```

5.5 Finalization

This part of the input file is finalized with the #5 end of fifth data group indicator.

6 Loads and withdrawals

This is the sixth group in the input file. This group may read like:

```
  19     ;  Number of loads and inflows
   8 'Ca. Bianca/Altipiano' 'Casa Bianca / Altipiano  ' 'Casa    '
  61 'Scolo Scarpion      ' 'Scolo Scarpion          ' 'Scolo   '
 143 'Scolo Altipiano     ' 'Scolo Altipiano         ' 'Scolo   '
 ...     ......                ......                    ...
2622 'Idrovia Veronese    ' 'Idrovia Veronese        ' 'Idrovia'
2642 'Ca. Deriva          ' 'Casa Deriva             ' 'Casa    '
2706 'Fiume Vallio/Cle.d.V' 'Fiume Vallio/Cle de Veneto' 'Fiume  '

   CONCENTRATION   FLOW
   ITEM       1     2     3
   DATA      0.84  0.9   2.6

   ITEM   'Ca. Bianca/Altipiano'
          'Scolo Scarpion       '
          'Scolo Altipiano      '
   CONCENTRATION
          Continuity
          Oxy
          PO4
      USEFOR   AAP   Tot-P – PO4  MIN  0.0
   TIME  LINEAR   DATA
                    Continuity  Tot-P  PO4   Oxy
   2005/01/01-00:00:00  1.0      0.4   0.25  7.5  ;  load 1
                        1.0      0.6   0.31  6.5  ;  load 2
                        1.0      0.37  0.16  8.3  ;  load 3
        .....    .....   .....
   2006/01/01-00:00:00  1.0      0.56  0.33  8.3  ;  load 1
                        1.0      0.42  0.23  6.7  ;  load 2
                        1.0      0.58  0.27  8.1  ;  load 3
      ITEM
          .....   ......

  #6            ; delimiter for the sixth group of input data
```

6.1 General

This is the sixth group in the input file. Waste loads are an external forcing to the system in the form of added (or withdrawn) masses. They can be associated with point sources as well as diffuse sources. There are similarities with open boundaries. Waste loads however distinguish in some important aspects from open boundary conditions:

◇ Loads and withdrawals do not play a role in the numerical solution of the substances transport. They just add (or subtract) mass from computational cells. There functioning is not contained in the 'from'-'to' pointer table for exchanges between the finite volumes.

◇ Loads and withdrawals are internally always expressed as mass/unit of time. Externally they may be specified as a flow with a concentration, but alternatively also directly as mass/unit of time. There need not be a flow associated with the waste loads.

◇ If a load flow is substantial enough to be contained in the hydrodynamic model result, then it depends on the coupling program with the hydrodynamic model whether that flow becomes available for D-Water Quality input processing. For Deltares software, the supported flow modules write files with flow information from point sources or distributed sources. These files can directly be used by D-Water Quality for its input processing and only concentrations need to be attached.

◇ If a load flow is contained in the hydrodynamic model, but if the hydrodynamic model does not make an input file for D-Water Quality to obtain that flow, then you can instruct D-

Water Quality to compute the flow from the closure error in the hydrodynamics dataset at that location. This requires that each computational cell has at most 1 waste load. If there were more for one cell, then there is only one closure error and it is impossible for D-Water Quality to determine which share of the error belongs to which load.

◇ If a withdrawal has to withdraw water with the current model concentration, then this is done through the specification of the withdrawal flow.

◇ Specific options exist to support the treatment of distributed or diffuse sources.

◇ Loads are specified for all substances, so also the non-transported, inactive substances. Open boundary conditions are only accepted for transported, active substances

Note: The loads and withdrawals are applied explicitly for all solvers. This means that especially for withdrawals a maximum time step applies to avoid instabilities at the location of the withdrawal. The maximum time step size should at least be less than the volume of the segment of withdrawal divided by the withdrawn flow. In the near future it may be expected that for implicit solvers also the process of withdrawing water will be implemented in an implicit way in order to eliminate this stability constraint.

6.2 Number of loads and identification of loads

The first required information is the number of loads. Subsequently for each load identification is required. The load identification consists of:

◇ the computational cell number where the load occurs. This cell number is generally easy determined by clicking the cell in the Graphical User Interface.

◇ A load-ID. The first 20 characters of the load-ID should be unique.

◇ A load-name. This input is not used by D-Water Quality but assists the user in the identification of the load entry also in mass balances. The first 40 characters are echoed to the listing file.

◇ A load-type. The first 20 characters of the load type are recognized and can be used to group the load entries e.g. to the type 'Agriculture'. For all entries of a type, one identical concentration can be specified.

It is possible to specify empty strings for all entries. The net effect of this specification will be that D-Water Quality fills in strings for the entries itself. This is generally not so informative and also not so convenient.

6.2.1 Special loads

Instead of a cell number you may specify one out of 3 keywords:

◇ SURFACE
This will produce a waste load proportional the surface of the cell, for each computational cell that has a water surface. It is meant to support the effect of rain and/or evaporation. This special waste load requires the presence of a parameter or segment function with the ID SURF. Specified values are $/m^2$.

◇ BANK
This will produce a waste load 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. Specified values are $/m$.

◇ BED
This will produce a waste load proportional to the horizontal surface area for each computational cell that has a water bed underneath. It is meant to support the effect of well and sink. This special waste load requires the presence of a parameter or segment function

with the ID SURF. Specified values are $/m^2$.

These keywords come instead of a cell number, and must always be followed by either MASS or CONC (see Load entry options in 6.2.2). The consequence is that all cells that have a surface, have a bank or have a bed are affected by this waste load specification. The ID, name and type string are still required to identify the load in the further specification blocks.

6.2.2 Load entry options

You may optionally precede the waste-load-ID with one of 4 keywords:

◇ MASS
This indicates that the information that follows for this load is to be considered as mass/unit of time (generally g/s). Any also specified FLOW value will not be used.

◇ CONC
This indicates that the information that follows for this load is to be considered as concentration (generally g/m^3). Flow information is now required to obtain waste loads other than zero for this option.

◇ RAIN
This indicates that the specified concentrations should be used by D-Water Quality if the flow is positive and that zero concentrations should be used if the flow is negative (like for evaporation).

◇ WELL
This indicates that the specified concentration should be used if the flow is positive and that the model concentration should be used if the flow is negative (like for groundwater abstraction).

If the keywords are missing, then the default waste load processing of D-Water Quality applies. This default load processing consists of:

◇ No flow is specified or the specified flow is exactly zero:
Then all values for the substances are considered to be expressed in mass/unit of time (generally g/s).

◇ 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.

◇ The specified flow is negative:

  □ If concentrations are not zero, the specified concentrations are withdrawn.
  □ If concentrations are zero, the model concentrations will be withdrawn.

This default behavior is tricky for a number of reasons. If e.g. a specified time series for the flow contains zero values then suddenly, within the time series, the specified concentration would be interpreted as a mass. The same type of sudden shift in behavior would appear with withdrawals when the concentration becomes zero within a time series. Finally if flow and / or concentration values are specified as time series and are linearly interpolated, then it becomes increasingly difficult to identify when the value becomes zero and what the actual load will be. Sometimes a small non-zero flow value of e.g. 1.0E-20 is included to force the values to remain concentrations rather than mass. To avoid this ambiguity, the keywords are introduced to give the user full control. Please note that the keywords apply per waste load, so not for all together, but also not per substance or per input block.

6.3 Concentration values

If you specify furthermore nothing, then zero will be used as load mass or concentration for all substances and all load entries. Everything that you specify here will fill in just the entry that you specify. If you specify the same entry and the same substance twice, then the last specification will be used. If you first specify a high frequency sampled time series for an entry-substance combination and later on a lower frequency sampled time series for the same entry but for a combination of that entry with other substances, then both are applied. This means that you are fully flexible. The specification of concentrations is done through a number of input blocks, each containing the concentration values for a number of waste load entries and a number of substances.

6.3.1 A 'substance' called FLOW

This load processing section also recognizes a substance-ID called `FLOW`. The information gathered under this ID will be used as the flow associated with the load. If this `FLOW` information is missing for a certain load then a value of zero is used for the flow of that load. The dimension of flow is m^3/s. This means that if you specify flow for a `SURFACE` or `BED` load, the dimension becomes m/s because it is multiplied with the `SURF` parameter that has dimension of m^3/s. You may convert existing tabular values of rainfall data expressed in mm/day to the required m/s unit by e.g. specifying a scale factor of 10-3 / 86400 = 1.1574E-08 in the D-Water Quality input.

As indicated earlier you may specify -999.0 to indicate a missing value. If you do so for the `FLOW` then something special happens. If the load is contained in the hydrodynamic dataset, then D-Water Quality will compute the flow from the closure error in the hydrodynamics of the grid cell of the load. This requires that at most 1 load exists for a grid cell, because only one closure error can be computed per grid cell. If the flow is not contained in the hydrodynamic dataset then the closure error computation will automatically produce a zero value.

6.3.2 Input blocks

The input is organized in blocks. Each block consists of the definition of the entries that are specified in the block, these are called `ITEM`. Furthermore the block definition consists of the substances that are specified in the block, they are called `CONCENTRATION`. The `DATA` in a block consist of a (series of) matrix(ices). If you first specified the `ITEM` entries, then the matrix consist of rows of concentration values. One for each item. If you first specified `CONCENTRATION` entries, then the matrix consists of rows per substance and values for the items on the rows. Be aware that D-Water Quality reads tokens only. D-Water Quality is not aware of the layout that you use for the input file. You may put all your information on one line, or you may put every item on a subsequent line. You cannot leave a matrix entry blank and you cannot assume that a new row starts with a new line. A new row starts if enough data is read for the previous row. So if there is no value available, then you may specify -999.0 instead. This is interpreted by D-Water Quality as a missing entry.

Character strings may be embedded in single or double quotes. Quotes / double quotes are only required if there are embedded blanks or embedded quotes in the string.

So either:

```
ITEM
   'Amsterdam wwtp'
   'Rotterdam harbor'
CONCENTRATION
   FLOW
   Ecoli
   Oxygen
DATA  ; flow m3/s  EColi      oxygen
```

```
                            1.2      1.0E+08          7.5         ;   Amsterdam wwtp
                            3.1      0.5E+06          8.4         ;   Rotterdam harbor
```

or:

```
CONCENTRATION
   FLOW
   Ecoli
   Oxygen
ITEM
   'Amsterdam wwtp'
   'Rotterdam harbor'
   DATA  ;      'Amsterdam wwtp'     'Rotterdam harbor'
                     1.2                    3.1            ; FLOW
                   1.0E+08                 0.5E+06         ; Ecoli
                     7.5                    8.4            ; Oxygen
```

6.3.3 Column headers and computations

Within one or more input blocks you may apply column headers that are no comments in the following way:

```
ITEM
     Agriculture
     Woods
CONCENTRATION
   USEFOR   Continuity     Cont
   USEFOR   Oxy            O2
   USEFOR   PO4            Tot-P  -  Part-P  MIN  0.0
   USEFOR   AAP            Part-P
DATA
   Cont   Tot-P Part-P  NO3-N   O2
   1.0    0.15   0.1    1.7    7.5   ;  Agriculture
   1.0    0.05   0.03   0.5    8.4   ;  Woods
```

Now the column headers are used as an identification of the column. They need not correspond with the reserved names of the processes library, but they can be linked through the `USEFOR` clause.

◇ Note that the order of the columns is not important.
◇ Note that the NO3-N column is not used.
◇ Note that computations are possible:

  ▢ The tokens and computational symbols should be separated by one or more blanks
  ▢ `+`,`-`,`*`,`/`, MIN and MAX are possible as computational directives
  ▢ They are evaluated in agreement with accepted math rules, i.e. `*` and `/` are evaluated before `-` and `+`. Brackets can not be used. If you want a*(b+c), then you should specify `a * b + a * c`.
  ▢ Instead of a column header token also a number can be used in the computations
  ▢ The computations act on whole columns, so if your columns are items, then the computations may be less useful

6.3.4 Time series

Time series start using the `TIME` keyword before the `DATA` keyword. This tells the input processor that this input block consists of a time series. Once you specified this keyword, D-Water Quality expects a series of matrices rather than a single matrix. The most simple

time series consists of 2 matrices for 2 time stamps. Each matrix should be preceded by a 'time'. This can be:

⋄ An integer in `DDHHMMSS` format if you specified to use that format in the group 1 input section.
⋄ An integer in seconds if you did not specify to use the format.
⋄ If you gave a reference time in the model ID strings in the group 1 input section, then you can also specify calendar dates here as e.g. `2012/02/28-12:35:00`. The two '/', the '-' and the two ':' characters are required exactly in this form, otherwise the time string will not be recognized.

D-Water Quality reads sets of a time and a matrix of data untill it meets a reserved keyword (mostly `ITEM` or `CONCENTRATION`) that starts the subsequent data block. Also the `#6` end of data group 6 signal ends the processing of a time series.

6.3.5 Linear interpolation

The default processing of time series is that the specified value at a specified time in used up to the next specified time. Then the value switches to the next specified value, a so-called block wave. For one or more of the input blocks you may alternatively want to interpolate linearly in between two specified values at specified times. To make D-Water Quality interpolate your time series linearly, you insert `LINEAR` after the `TIME` keyword and before the `DATA` keyword. Also the `BLOCK` keyword is supported, but it is superfluous since this is the default processing of time series.

6.3.6 Scale your input

If you copy and paste large amounts of data into your input file, then it is cumbersome if the data does not have the units that are required for the simulation. If you have data in $mole$ or in $\mu g/l$ rather than the g/m^3 or mg/l that is required by D-Water Quality then it is convenient that you just scale your input. You do so by specifying the `SCALE` keyword before the `DATA` keyword. The `SCALE` keyword should be followed by as many scale factors as there are columns in the matrices that you will provide. So you must provide 1.0 for each column that will not be scaled. A scale factor can be especially useful for loads through rainfall if you have rain data in mm/day whereas you have to provide your input in m/s. Also concentration data for coliforms (`MPN/100 ml`) generally need to be converted. Alternatively the `USEFOR` with multiplication can be used to scale the input.

6.3.7 Data from external non-ASCII files

D-Water Quality supports the entry of data from non-ASCII self describing so called `ODS_FILE` files. This Deltares proprietary file format is not further documented here. The use of this option is to specify the `ODS_FILE` keyword followed by the name of the file. This specification is used instead of the `DATA` keyword and the data matrices that follow that keyword.

6.3.8 Multiple copies of substances

If the feature of multiple copies of substances is used, then for each copy a load must be provided. This is facilitated by the input structure through e.g.:

```
ITEM              'Rotterdam WWTP'
CONCENTRATIONS
    USEFOR  TColi01   Coliforms   * 0.25
    USEFOR  TColi02   Coliforms   * 0.25
```

```
      USEFOR  TColi03   Coliforms   * 0.50
TIME LINEAR
DATA                  Coliforms
1990/08/05-12:30:00   1.00e+009
1990/08/06-01:00:00   1.20e+009
```

6.3.9 Useful options

◇ Use different groups for flow and concentrations
Often the flow is available as a time series with e.g. a value per day, whereas the concentrations may be constant or have a value each month. If you put the flow in one block and the concentrations in another block, each with there own number of time values, then D-Water Quality will evaluate the flow and concentration independently per time step and then multiply them at run time to obtain the load.

◇ Group waste load concentrations for a specific class of loads
With the above procedure it is easy to provide e.g. the waste load concentrations for many loads of a certain class like 'agriculture' in one block. With the directive
`INCLUDE "..\data\agriculture.dat"`
you can retrieve that information from a separate file.

◇ Separate time varying concentration data and constant concentration data
You just place them in different blocks.

6.3.10 Internal intelligence

To assist you in providing the input, you can best pose yourself the question: "how does DELWAQ knows?".

◇ If you say `ITEM` then D-Water Quality expects strings with items. It signals if such a string is neither an item (a load or a load type) nor a new keyword.

◇ If you say `CONCENTRATION` then any pending procedure for item processing stops and the procedure for substances starts. It signals if your substance entries are not recognized as model substances and the entry is also not a new keyword. `USEFOR` is allowed, but should be followed by a character token that is found as column header and optional computational instructions. If a computational operator (+, -, *, /, MIN, MAX) is followed by a character token, then the new character token should either be a new column header or a recognized keyword.

◇ If you say `DATA` then data should follow. If you however specified `TIME` before, then first a 'time' stamp should be provided. That can be an integer or a calendar time string. If the first time stamp is a character token that is not an absolute time string, then D-Water Quality assumes that you started to provide column headers.

◇ If you specified a matrix of input data, then either an integer time or a calendar time string should follow, followed by the next matrix or a new keyword should follow to end the input block and start a new input block.

6.4 Finalization

This part of the input file is finalized with the `#6` end of sixth data group indicator.

7 Process steering

This is the seventh group in the input file. This input group may read like:

```
    CONSTANTS        'ONLY_ACTIVE'            DATA  1.00000e+000
    CONSTANTS        'ACTIVE_VarSal'          DATA  1.00000e+000
    CONSTANTS        'ACTIVE_BLOOM_P'         DATA  1.00000e+000

    PARAMETERS       'SURF'      ALL      BINARY_FILE 'SURFACE.FIX'

    FUNCTIONS        'VWIND'    LINEAR        DATA
;    dddhhmmss
       000000000        3.44E+00        ; Begin year
       182120000        2.10E+00        ; Half way
       365000000        4.44E+00        ; End year

    SEG_FUNCTIONS  'Temp'      ALL     BINARY_FILE 'hydrodyn.tem'

    CONSTANTS        'Dry_THresh'            DATA  0.25
    CONSTANTS        'NOTHREADS'             DATA  0

#7           ; delimiter for the seventh group of input data
```

7.1 General

The water quality processes make the model to a water quality model. They are 'objects' in
the sense of the 'Component Software' philosophy. It is important for the user to know that
there are 2 modes for the processes:

1 They are switched on automatically by D-Water Quality with internal inference rules.
2 They are switched on by the user.

Because of unwanted side effects, method 1 is hardly used any more and this manual will
assume the use of method 2.

The user generally starts the PLCT (Process Library Configuration Tool). That is part of the
Graphical User Interface. This is a multi-level user interface to select substances, processes
and process steering that will be provided by the user rather than using the defaults for the
process. The PLCT also enables the selection of candidate extra output variables. These are
generally intermediate computations (like total biomass, total suspended solids etc. from the
fractions). They can also be meaningful derived variables like Chlorophyll, whereas the pro-
cesses library models algae as Carbon and Secchi depth whereas the model uses extinction
coefficients.

The result of the PLCT selection process is a readable '*.sub' file. This file is ingested by the
user interface. In the user interface the user attaches his process steering to the items that
were selected with the PLCT. In the user interface the user also selects which of the candidate
output variables he really wants to include in what output files. The user interface generates
a D-Water Quality input file. This documentation describes the process steering part of the
D-Water Quality input file with the aim to allow the user to modify this section of the input file,
using options that are not available through the user interface. It is generally very useful to
have an existing input file or a user interface produced input file as starting point. It is very
tedious to construct this part of the input file without using the PLCT, because the *.sub file
as produced by the PLCT will list the processes IDs, the substance IDs and the IDs of the
selected input and output variables by their reserved character string. The only alternative is
to select them manually by running through the technical reference manual of the processes
library and copying the IDs that are mentioned there into the input file. It is advised to only
use the manual for details on specific processes rather than to construct this section of the
input file fully from the manual.

7.2 Steering items

The D-Water Quality input file distinguishes four different types of items:

◇ CONSTANTS
   These are single values that act during the whole simulation for each computational grid cell. Constants are generally used to provide the model with coefficients like partitioning coefficients for micropollutants. They are also used to provide the model with switches, flags and settings that may influence the computational procedure.

◇ PARAMETERS
   These are items that retain there value during the whole simulation but that may be different per grid cell. The elevation of the bed below reference level could be an example.

◇ FUNCTIONS
   These are items that have the same value for all grid cells, but that may vary during the course of the simulation. The annual pattern of solar radiatiation on the model may be an example of this type of input.

◇ SEG_FUNCTIONS
   These are items that vary in time and that may have different values per grid cell. They are called "segment function" in D-Water Quality terminology. This is huge information for a detail 3D model with many time steps. This information is generally produced by other software and attached as a file to this simulation. The temperature, salinity and suspended sediment concentration as computed by the hydrodynamic model are of this type, but also the vertical diffusion coefficient from the hydrodynamic model, that will be used in the D-Water Quality simulation is of this category.

It is important to realize that any steering item for process behavior can be any of these four types. For one simulation the temperature can be fixed both in time and all over the place. It will then be among the CONSTANTS. For another simulation it can be prescribed as an annual time function that is the same for each grid cell. It will then be among the FUNCTIONS in the input. For yet another simulation a spatial field of temperature values can be used and you will see it in the PARAMETERS input part. The temperature steering can also vary per time step and per grid cell and be among the SEG_FUNCTIONS. An example for the latter is e.g. the temperature file that is computed by a 3D hydrodynamic stratification model. Which type of input is used for a certain simulation is up to the user, the processes library automatically deals with any selection the user makes.

A steering item can also be part of the D-Water Quality simulation, the water depth of a grid cell is an example, but also the temperature can be computed by D-Water Quality itself rather than being provided as external steering. If this is the case the user does not need to do anything, D-Water Quality automatically attaches the model information to the process. For temperature this means that de D-Water Quality modeled temperature is used unless temperature is specifically provided as external steering by the user. In the latter case, the user specification of the external steering overrules the presence as state variable.

7.3 Data blocks

To assist the user, it is possible to provide the model steering in data blocks. Each data block contains just one type of data, so either `CONSTANTS`, `PARAMETERS`, `FUNCTIONS`, or `SEG_FUNCTIONS`. You can provide as many data blocks as you want, so it is possible to group certain functions by providing them in 1 block, or to supply them each in their own block. The order of the information in the input file does not matter. It is possible to start with a block of segment functions to continue with a block of parameters, to provide a block of constants and then again to provide a block of segment functions. Because you can use the `INCLUDE <filename>` directive anywhere in the file, you can use a separate file with steering coefficients from different sources of information, like meteorology or a certain measured dataset. In the following the 4 types of data blocks will be documented further.

7.3.1 CONSTANTS

To enter constants, you write `CONSTANTS` in the file. Then you write the IDs of the items that you want to provide as constants. The IDs must correspond exactly with the reserved names of the processes library, but they are not case sensitive. In the most simple case a collection of IDs is followed by the keyword `DATA` and then the values of the constants follow. You will find for example input like:

```
CONSTANTS
    SWresusalg
    SWAdsP
    KdPO4AAP
    MaxPO4AAP
    RcAdPO4AAP
    pH
DATA
    1.00000e+000 ; SWresusalg
    0.00000e+000 ; SWAdsP
    1.00000e+000 ; KdPO4AAP
    5.00000e-003 ; MaxPO4AAP
    5.00000e-001 ; RcAdPO4AAP
    8.20000e+000 ; pH
```

But since you can insert an arbitrary number of data blocks, you could equally well use:

```
CONSTANTS    SWresusalg DATA  1.00000e+000
CONSTANTS    SWAdsP     DATA  0.00000e+000
CONSTANTS    KdPO4AAP   DATA  1.00000e+000
CONSTANTS    MaxPO4AAP  DATA  5.00000e-003
CONSTANTS    RcAdPO4AAP DATA  5.00000e-001
CONSTANTS    pH         DATA  8.20000e+000
```

If the specified constants are resolved, the D-Water Quality input processor requires either a keyword that starts the next data block or the `#7` to end this group of input.

7.3.1.1 Special constants

There are some special constants. Some of them are only checked for their presence, so then the value of the constant plays no role. Others are used to give D-Water Quality one or more values that are used in its simulation process without affecting the water quality processes. The special constants are listed here:

⋄ constants that switch processes on
   If the constant `ONLY_ACTIVE` is present in the list of constants, then D-Water Quality is

using only those processes that are explicitly switched on. Otherwise D-Water Quality tries to figure out itself which processes it will switch on. This automatic procedure has however a number of unwanted side effects so it is hardly used any more. Processes are switched to 'on' furthermore by the presence of a constant `ACTIVE_proc_name`. *It does not matter what value is attached to the constant*. The presence of the constant alone will switch the process 'on'. The constants in the sample input on constants are important for processes associated with adsorbed and soluble phosphorus (AAP and PO4). So you should not be surprised to see in the list of constants also entries like:

```
CONSTANTS   ONLY_ACTIVE        DATA   1.0
CONSTANTS   ACTIVE_AdsPO4AAP   DATA   1.0
CONSTANTS   ACTIVE_Sed_AAP     DATA   1.0
CONSTANTS   ACTIVE_Res_AAP     DATA   1.0
```

In most applications you will see that a data value of 1.0 is used, but the exact value does not matter. So also with the value of 0.0 the processes are switched to 'on'. It may be good practice for the readability of the input file, to use 1.0 for the 'on' switching. If you want to swicth a process 'off' temporary but leave the entry in the input file, then you just insert a comment character at the beginning of that line.

◇ closure error switch

If the hydrodynamic files are exhausted and the simulation continues, then D-Water Quality automatically rewinds the hydrodynamic files. Because the model volume at the end of the dataset may not equal to the model volume at the start, an inconsistency arises. The default approach to this inconsistency is that D-Water Quality preserves mass. This means that you see that the time series of concentration values make a 'hiccup' because of the discontinuous volume. If the `CLOSE_ERR` constant is present however, the time series of concentration values will remain smooth and D-Water Quality adapts the mass to cause a smooth concentration curve behavior. The amount of volume that has to be added or removed at the rewind of the hydrodynamic datasets in this case is displayed in the monitoring file. This feature may give rise to severe errors if a grid cell was temporary dry at the start and wet at the end of the hydrodynamic database or the reverse.

◇ constants associated with implicit solvers

A number of constants are associated with implicit solvers. Here they are listed together with their default values.

```
CONSTANTS   swprecond         DATA   3.0   ; preconditioner
CONSTANTS   maxiter           DATA   100.0 ; max nr iterations
CONSTANTS   tolerance         DATA   1.0D-7 ; tolerance
CONSTANTS   swscale           DATA   1.0   ; row scaling
CONSTANTS   novec             DATA   50.0  ; Krilov space size
CONSTANTS   "iteration report" DATA  1.0   ; iteration report
```

The default for preconditioner is "lower and upper" tridiagonal, other values are 0 for "none" and 1 or 2 for "lower" or "upper" alone. The default for row scaling is 'on'. Use 0.0 to switch it 'off'. The Krilov space size may prevent the model to fit in 2GB of memory. The value may then be reduced to 25. It is not advisable to reduce it further. The default for the iteration report is 'on' and output is written to the monitoring file, but in many input you will find this constant with the value 0.0 and then it is switched 'off' to avoid bulky output.

◇ Parallel computing

D-Water Quality supports parallel computing on multi core PC's. This feature is generally switched 'off'. If you are confident with your model, you may switch it 'on' by giving:

```
CONSTANTS   nothreads   DATA   0.0   ; OMP-parallelism 'on'
```

With a value of 0.0 D-Water Quality will itself determine how many threads can be used. With a positive value you determine the number of threads. The default is -1.0 which means 'off'. Implicit solvers need a Krilov space for each thread. This can become large for e.g. 6 core PC's with hyper-threading featuring 12 threads. Then you better use a smaller positive number for the number of threads than the allowed number of 12 that you will get with a value of zero.

◇ Z-layer model processing
Hydrodynamic models in 3 dimensions using strictly horizontal layers, so called Z-layers, may feature a water surface that travels through layer interfaces when water level rises or falls like in dammed lakes. You will then need:

```
CONSTANTS ACTIVE_Emersion DATA 1.0  ; switches process 'on'
CONSTANTS ZThreshold      DATA 0.01 ; threshold in m.
```

This switches the Emersion process on. This process joins the top layer with the layer underneath if layer thickness is lower than ZThreshold and makes the new layer the top layer. At flooding the reverse happens. If the thickness is over 'ZThreshold' more than the thickness of the layer underneath, then a new top layer is formed. If you are not using this process, unpredictable results may occur for incomplete water columns.

◇ Z-layer model initial conditions
It is difficult, especially for bigger models, to manually specify initial conditions for bed variables in Z-layer models, because you generally do not know at what level the first wet cell appears. The solution is to specify initial conditions for bed variables (non-transported substances) in the lowest layer irrespective of whether it is below the bed or not. Furthermore you specify the constant `Z_Thresh` with a value of e.g. 0.001. Then all cells with a waterlayer thickness of 1 mm or below will be considered located below the bed. Those cells are set inactive, the initial condition is set to zero and the specified value is migrated upward until the first wet cell of the water column is reached.

◇ Drying and flooding
The way a hydrodynamic model administrates its drying and flooding is sometimes not fully clear to D-Water Quality. To ensure some basic safety, D-Water Quality has itself also a drying and flooding detection mechanisms to ensure that the volume of its computational cells will not fall to zero or even below zero. D-Water Quality will use a default threshold of 0.001 m or 1 mm. Below this water level a cell is considered to have ran dry. You can change this default value by specification of a constant with the name `DRY_THRESH` and giving it a value other than 0.001. The value is multiplied with the value of the horizontal surface area of the horizontal computational cells to obtain the threshold per water collumn locally in m^3. If no constant or segment function with the name `SURF` is found, then D-Water Quality cannot determine the threshold volume in m^3 by multiplication with `SURF`. For that situation the value of the constant `DRY_THRESH` is directly interpreted as a value in m^3 and the default value if no constant `DRY_THRESH` is found amounts to 1.0 m^3. Please note that the procedure is used for the whole water column, so not for the cell at one layer. This reflects the fact that either the water column ran dry locally or it is wet. Except for Z-models (see the item above), individual cells in a 3D model cannot run dry, the column does.

◇ Time step multiplier for the `BLOOM` process
The algae competition module `BLOOM` is generally operated on longer time spans than the remainder of the water quality processes. For many water quality processes a time step size of half an hour would do. A common time step size for the `BLOOM` process is a day. This requires:

```
CONSTANTS TimMultBL  DATA  48.0  !  factor from 0.5 hour to a day
```

You should be aware that when you need this constant that you have to adapt the constant as soon as you are changing the integration time step size for the other processes.

7.3.2 PARAMETERS

The keyword PARAMETERS is followed by a list of one or more parameter IDs. The IDs must correspond exactly with the reserved names of the processes library, but they are not case sensitive. If later on column headers are used and/or the parameter values are modified by computational instructions, then the USEFOR construct as described for boundaries and waste loads also applies here. This list ends if a reserved keyword is met. Valid reserved keywords are:

◇ DEFAULTS, ALL, SEGMENTS, INPUTGRID
These keywords are associated with definition of the way the data will be attached to the computational cells, the segments.

　□ DEFAULTS
　With this keyword it is expected that for each parameter one value will follow. This value will be used for all segments.
　□ ALL
　With this keyword it is expected that for each parameter and each segment a value will be given.
　□ SEGMENTS
　With this keyword it is expected that a list of segment numbers will follow for which the parameter values will be specified.
　□ INPUTGRID
　With this keyword it is expected that the name of an earlier defined grid is mentioned. The parameter values will be given for the cells of this grid and will then be expanded to other grids when needed by D-Water Quality.

◇ BINARY_FILE or UNFORMATTED
This keyword indicates that the mentioned parameters will be retrieved from a binary file or an unformatted file (which is a binary file with special FORTRAN compiler depending structure of records). This keyword should be followed by the file name. The parameters are expected to be located in the file in the order of their appearance in the list that was just closed by the keyword. First all parameters for computational cell 1 are expected, then all for cell 2 etc.

◇ BIG_ENDIAN
This keyword indicates that the binary file or unformatted file has its data in BIG_ENDIAN structure. This structure is common for files on mainframe computers and on some massive parallel computers. BIG_ENDIAN files are also produced by the TELEMAC hydrodynamic models.

◇ ODS_FILE
This is a sort of self descriptive proprietary Deltares file format that is not further documented here. This keyword should be followed by the file name of the file.

◇ DATA
This keyword starts data entry. It will produce an error if not first the segments are defined where the parameters will be given for. So first one of the keywords ALL, DEFAULTS, SEGMENTS, INPUTGRID is expected with associated additional information if that is needed for the keyword.

　□ For DEFAULTS, as many values are expected as there are parameters in this block.
　□ For SEGMENTS, all parameters of this block are expected for all segments that were mentioned by number after the SEGMENTS keyword.
　□ For INPUTGRID, all parameters of this block are expected for all segments of the mentioned input grid.
　□ For ALL, all parameters of this block are expected for all segments of the model grid. This is the biggest file and is often produced by the hydrodynamic model or by the user interface, but you could of course yourself also specify 2345*3.1 9380*2.8 2345*2.4

for 1 parameter in a 6 layer model with 14070 grid cells.

Like with boundary conditions and loads, the data may be preceded by column headers displaying the names of the columns in the input file. If information comes from a binary or unformatted file, then the parameters are expected in the order in which they are mentioned in this block. First all parameters for segment 1, then all parameters for segment 2 etc.

A sample input for a parameters block can e.g. consist of:

```
PARAMETERS
    Surf
    Bottomdept
ALL
BINARY_FILE BIG_ENDIAN  '..\data\Bodensee.par'
```

but also of:

```
PARAMETERS 'fixth'  INPUTGRID 'sediment-zone'
DATA  0.001   ; layer 1
      0.002   ; layer 2
      0.003   ; layer 3
      0.006   ; layer 4
      0.018   ; layer 5
      0.07    ; layer 6
      0.1     ; layer 7
PARAMETERS  'SURF'
      INPUTGRID 'water-grid'    BINARY_FILE  'surf.par'
PARAMETERS  'SURF'
      INPUTGRID 'sediment-grid' DATA INCLUDE 'surf-sediment.dat'
```

Note that by the last 2 specifications the water-grid gets its horizontal surfaces from a file coming through the user interface from the hydrodynamic model and that additionally the horizontal surfaces of the much coarser sediment-grid with the layered water bed come from a readable `ASCII` file that is included here.

7.3.3 FUNCTIONS

The keyword `FUNCTIONS` is followed by a list of one or more function IDs. The IDs must correspond exactly with the reserved names of the processes library, but they are not case sensitive. If later column headers are used and/or the function values are modified by computational instructions, then the `USEFOR` construct as described for boundaries and loads also applies here. This list ends if a reserved keyword is met. Valid reserved keywords are:

◇ `LINEAR, BLOCK`
These keywords indicate the interpolation mechanism to be used for the functions between the specified points. `BLOCK` is the default procedure, so that keyword is superfluous.

◇ `HARMONICS`
This keyword indicates that harmonic functions will be specified. These functions are not interpolated, but analytically evaluated according to:

$$f_t = f_{average} + \sum_{i=1}^{n} \left(amplitude_i \cdot \sin \left(\left(\frac{t}{period_i} - phase_i \right) \cdot 2\pi \right) \right)$$

◇ FOURIERS
This keyword indicates that Fourier functions will be used. These functions are not interpolated, but analytically evaluated. The analytical formula is the same as for harmonics with the distinction that there is a base period for the first component and that $period_i = baseperiod/i$ with i the component number.

◇ TIME_DELAY
This keyword indicates that the times of the functions specified should be delayed with a certain amount of time. It is followed by the time delay value that is an integer in units of the system clock (generally seconds) or an integer in DDDHHMMSS or YYDDDHH format if that format was previously selected for input of times. The time delay value allows the use of unaltered datasets from other years or months for the model years or months. The alternative would be to edit the time strings in those files to make them fit for the different year. It should be anticipated that a day could be lost or should be interpolated at the end of some February months.

◇ BINARY_FILE, UNFORMATTED, ODS_FILE
These keywords are not common for functions and they are even not allowed if the use of HARMONICS or FOURIERS is specified.

◇ DATA
This keyword starts data entry. Expected is:

□ optional column header strings for the columns that will follow. De input processor will then select the appropriate columns and will skip the non used columns.

□ for normal time series specified at breakpoints, the input processor expects a sequence of:

○ a time integer or an absolute calendar time string
○ the function values at that time in the order of the list of this block or according to the column headers

□ for HARMONICS functions, the input processor expects:

○ the $f_{average}$ values for the functions in the order of the list of this block.
○ as many sets of input as there are harmonic components with:

▷ a time interval integer for this harmonic component in units of the system clock giving the $period_i$ of harmonic component i.
▷ a real value between 0 and 1 or between -0.5 and +0.5 for $phase_i$ of this harmonic component with respect to the start of simulation
▷ the $amplitude_i$ values of this harmonic component for the functions in the order of the list of the block

□ for FOURIERS functions, the input processor expects a sequence of:

○ a time interval integer in units of the system clock giving the $baseperiod$ of this Fourier series.
○ the $f_{average}$ values for the functions in the order of the list of this block.
○ as many sets of input as there are Fourier components with:

▷ a real value between 0 and 1 or between -0.5 and + 0.5 for $phase_i$ of this Fourier component with respect to start of simulation
▷ the $amplitude_i$ values of this Fourier component for the functions in the order of the list of the block

Data entry ends when either a keyword is met that opens a new input block or when the #7 is met to end this group of input.

7.3.4 SEG_FUNCTIONS

The keyword `SEG_FUNCTIONS` is followed by a list of one or more segment-function IDs. The IDs must correspond exactly with the reserved names of the processes library, but they are not case sensitive. This list ends if a reserved keyword is met. Valid reserved keywords are:

◇ `LINEAR`, `BLOCK`
These keywords indicate the interpolation mechanism to be used for the segment-functions between the specified points. `BLOCK` is the default procedure, so that keyword is superfluous.

◇ `TIME_DELAY`
This keyword indicates that the times of the functions specified should be delayed with a certain amount of time. It is followed by the time delay value that is an integer in units of the system clock (generally seconds) or an integer in `DDDHHMMSS` or `YYDDDHH` format if that format was previously selected for input of times. The time delay value allows the use of unaltered datasets from other years or months for the model years or months. The alternative would be to edit the time strings in those files to make them fit for the different year. It should be anticipated that a day could be lost or should be interpolated at the end of some February months.

◇ `BINARY_FILE`, `UNFORMATTED`, `ODS_FILE`
These keywords are very common for segment-functions because these are generally generated by other models. These keywords are generally followed directly by the file name of the file, but it is also possible to specify `BIG_ENDIAN` to indicate that the file is written with that file structure.

◇ `MULTIPLEHYD_FILE` followed by the file name of such a file. See the annex of this manual for the description of multiple hydfiles.

◇ `DATA`
ASCII input of segment-function time series specified at breakpoints is rare, because this information is generally voluminous. Should it nevertheless occur then the input processor expects a sequence of:

□ a time integer or an absolute calendar time string
□ the function values at that time in the order of the list of this input block. Unlike e.g. parameters, this data is required as: for all computational segments the values of segment function 1; for all computational segments the values of segment function 2; .... etc.

Data entry ends when either a keyword is met that opens a new input block or when the `#7` is met to end this group of input.

7.3.5 Multiple copies of substances

If the feature of multiple copies of substances is used, then all process data is duplicated automatically. You can however also specify fraction specific steering like in:

```
CONSTANTS  VsedIM1       DATA  1.0  ; holds for all fractions except:
CONSTANTS  VsedIM1*IM102 DATA  2.0  ; specific for fraction 02
```

7.4 Finalization

This part of the input file is finalized with the `#7` end of 7th data group indicator.

8 Initial conditions

This is the eighth group in the input file. This input group may read like:

```
      0            ; initials from binary restart file
   lpr001_res.map  ; name of the restart file
      #8           ; delimiter for the eighth group of input
```

This is *old-style* input to start from a restart file. It could also be:

```
    MASS/M2     ;    The bed substances are specified in mass/m2
      2         ;    Input with defaults
    23*1.0      ;    Scale values
;  Continuity Salinity    im1      im2      oxy      nh4    etc.
    1.00      24.00    5.00    0.00    6.50    0.15   ...
      2              ; number of overridings
    13816  ;  first overriding
    1.00       0.00    15.0    0.00    8.00    1.20   ...
    23456  ;  second overriding
    1.00       0.00     5.0    0.00    9.00    0.40   ...
```

This is *old-style* input to start from a set of prescribed initial values with exceptions for 2 cells. It could also be *new style* input especially suitable for models with a layered water-bed:

```
   MASS/M2                      ;  bed substances in mass/m2
   INITIALS    Continuity Salinity   im1      im2      oxy      nh4    etc.
   INPUTGRID   water-zone    ;  this grid was defined in input group 3
   DATA        1.00     24.00    5.00    0.00    6.50    0.15   ...

   INITIALS
 Continuity Bulkvolume Salinity   im1      im2      oxy      nh4     etc.
   INPUTGRID
 sediment-zone  ;   this grid was defined in input group 3
   DATA
    1.00   1.00   24.00    3.44E05   2.29E05   0.05   0.01   ... ; layer 1
    1.00   1.00   24.00    3.66E05   2.44E05   0.05   0.01   ... ; layer 2
    1.00   1.00   24.00    3.86E05   2.57E05   0.05   0.01   ... ; layer 3
  #8          ; delimiter for the eighth group of input data
```

8.1 General

Initial conditions should be given for all modeled substances and all computational volumes (segments). The initial conditions are given as a concentration value for all active substances that are transported with the water. D-Water Quality itself uses masses of the substances as state variables and the concentrations of the state variables are derived entities for output processing and for the evaluation of water quality process kinetics. This means that D-Water Quality will multiply the initial concentration values with the volumes of the segments to initialize its state variables for simulation. D-Water Quality also contains inactive substances that are not transported with the water because they are located on the water bed or because they are part of the layered water bed. In the past the latter type of substances had to be initialized directly by their mass per computational volume. That was very cumbersome because computational volumes could differ and are largely unknown to the user. The user is just using the output of a hydrodynamic model for volumes, areas and flows. Not so long ago this issue was resolved by using the unit $mass/m^2$ as 'concentration' unit for these non-transported substances.

A second major change in the processing of initial conditions was a consequence of the layered bed model. Now the user can define a layered bed underneath the water phase. But since the geometry of the water phase is generally determined by the hydrodynamic model that produces the water flows and turbulences, additional geometry needs to be defined for the bed. That is done in group 3 of the input file by the definition of a grid within the bed that is linked with the overlying water grid. In this group 8 of the input file we will see how variables within that grid in the water bed are initialized.

8.2 Old specification

This specification is not convenient for the layered bed model, but may still be convenient for simpler models.

◇ The `MASS/M2` directive (optional)
This directive is only useful if your simulation contains also passive, non-transported substances. With the directive you say that you will provide initialization for these substances in in the form of $mass/m^2$ rather than as $mass/gridcell$. The directive does not work for binary files (see below).

◇ An integer file switch (obliged)
This switch can have two values:

0 for an external binary file
This external binary file can be:

□ A so-called `.ini` file
This is an older type of initial condition file that is no longer produced, but may still be available as remnant from older runs. The file just contains a matrix of real numbers. D-Water Quality assumes that any passive substances in this file are given as $mass/gridcell$ because that was common when the file was written (most likely by the user interface.

□ A so-called `.res` file
This file is still produced as restart file by D-Water Quality | itself. It will be phased out soon and it is advised to not use this file any more. Produced by the newer D-Water Quality releases this file will contain the passive substances as $mass/m^2$. Produced by the older releases it contains the passive substances as $mass/gridcell$ and is identical to the `.ini` file.

□ The `runID_res.map` file
This file is now produced. It contains information that allows you to check its content with any graphical postprocessor of D-Water Quality results, because it is a standard D-Water Quality simulation result file with only one time step included: the result at 'end-of-simulation'. This file is presently also produced by the user interface and it contains information that allows D-Water Quality also to identify whether the passive substances are initialized as $mass/m^2$ or as $mass/gridcell$. Any necessary conversion is performed automatically.

1 for the ASCII input file
This ASCII input file will contain:

□ The `TRANSPOSE` directive (optional)
This directive allows the specification of the matrix of initial conditions in interchanged row - column order.

□ An integer switch (required)
This switch can have two values:

1. for input without default values
This integer should be followed by a scale value for each of the substances in the order that was mentioned in group 1 of the input data.

Then for all substances in the order that was mentioned in group 1 values should be given for all segments. First all values for segment 1, then all values for segment 2, ... and so on. For small models with not too many substances, this is still possible by e.g.:

```
        1        ;   Input without defaults
      23*1.0     ;   Scale values
 ;  Continuity Salinity    im1     im2     oxy     nh4    etc.
      1.00      24.00     5.00    0.00    6.50    0.15   ...
      .....     .....     ....    ....    ....    ....   ...
      1.00      24.00     5.00    0.00    6.50    0.15   ...
```

But for larger models with numerous grid cells, you may want to say:

```
    TRANSPOSE
        1        ;    Input without defaults
       1.0       ;    Scale value
  23764*1.00     ;  Continuity
  23764*24.0     ;  Salinity
  23764*5.00     ;  im1
  23764*0.00     ;  im2
  23764*6.50     ;  Oxy
  23764*0.15     ;  NH4
```

You can specify only one scale factor for all substances with the TRANSPOSE keyword

2. for input with default values e.g.

```
        2        ;    Input with defaults
      23*1.0     ;    Scale values
 ;  Continuity Salinity    im1     im2     oxy     nh4    etc.
      1.00      24.00    5.00    0.00    6.50    0.15
        2           ;  number of overridings
    13816  ;  first overriding
      1.00      0.00    15.0    0.00    8.00    1.20
    23456  ;  second overriding
      1.00      0.00     5.0    0.00    9.00    0.40
```

8.3 New specification

The more modern approach to providing initial conditions with ASCII input may still start with the MASS/M2 keyword to indicate that the bed substances are given in weight per m^2 rather than in weight per grid cell. The new specification itself then starts with the INITIALS keyword. This keyword triggers similar procedures as the PARAMETERS keyword in group 7 of input data does. This is best illustrated with the following example from a model with layered bed:

```
   INITIALS
Continuity Salinity   im1     im2     oxy     nh4     etc.
  INPUTGRID
water-zone      ;   this grid was defined in input group 3
  DATA
    1.00     24.00    5.00    0.00    6.50    0.15   ...

   INITIALS
Continuity Bulkvolume Salinity   im1     im2      oxy     nh4     etc.
  INPUTGRID
sediment-zone  ;   this grid was defined in input group 3
  DATA
;  layer 1
```

```
     1.00       1.00      24.00    3.44E05   2.29E05     0.05     0.01   ...
;  layer 2
     1.00       1.00      24.00    3.66E05   2.44E05     0.05     0.01   ...
;  layer 3
     1.00       1.00      24.00    3.86E05   2.57E05     0.05     0.01   ...
```

Here 2 input blocks are given, one acting for the 1 cell 'water-zone' and a second one acting for the 3 cell 'sediment-zone' that were defined in group 3 of the input file. These initial conditions are expanded automatically by D-Water Quality to all the grid cells that are contained in the mentioned zones. This example illustrates why this way is more convenient especially for the layered bed approach .

Both ways are likely to be continued in future releases, because once a simulation is made using a layered bed model, it remains convenient to initialize the next simulation simply with:

```
      0              ; initials from binary restart file
lpr001_res.map   ; name of the restart file
     #8              ; delimiter for the eighth group of input
```

8.3.1 Multiple copies of substances

If the feature of multiple copies of substances is used, then for each copy an initial condition must be provided. This is facilitated by the new input structure through e.g.:

```
INITIALS
    Salinity
    NO3
    USEFOR  Diat01   Diatoms   * 0.25
    USEFOR  Diat02   Diatoms   * 0.25
    USEFOR  Diat03   Diatoms   * 0.50
DATA   Salinity NO3    Diatoms
       16.0   1.0      0.5
```

8.4 Z-layer models

Z-layer models feature strictly horizontal layers, unlike sigma layer models that divide the water column in a certain fixed ratio. This means that the lowest water layer in sigma models is always the layer where the water bed is located. In Z-layer models this depends on the local water depth. It is difficult to specify initial conditions that are related to the presence of the water bed in Z-layer models, because detail knowledge is required on where the bed is located in every water column. To avoid problems, you just specify your initial conditions of Z-layer models for the cells with a water bed just as if you specified the initial condition for a sigma layer model, in the lowest model layer. You furthermore specify a constant `Z_Thresh` in your group 7 input with a value for the thickness in meters below which a cell should be considered dry. The D-Water Quality run-time processor will then start with migrating your prescribed values to the first wet cell from beneith in each column and zero out everything below. If you specify a restart file as initial condition then this problem will not occur of course, since then the restart values are defined in the correct cell and the run-time processor need not do anything. This automatic elevation of initial conditions is only performed for inactive substances.

8.5 Finalization

This part of the input file is finalized with the `#8` end of eighth data group indicator.

9 Model output

This is the ninth group in the input file. Input in this group may read like:

```
 1 ; output information in this file
 2 ; all substances and extra output for the monitoring file
11 ; number of extra variables
'NH3'           'volume'
'BOD5'          'volume'
'TotalDepth'    'surf'
'Chlfa'         'volume'
'SS'            'volume'
'DisCu'         'volume'
'TotN'          'volume'
'DIN'           'volume'
'TotP'          'volume'
'SURF'          ' '
'LocalDepth'    'surf'
 0 ; no output is required for the dump file
 2 ; all substances and extra output for the history file
11 ; number of extra variables
'NH3'           'volume'
  ....
'LocalDepth'    'surf'
 2 ; all substances and extra output
11 ; number of extra variables
'NH3'
 ......
'LocalDepth'
1 ; binary history      file 'on'
1 ; binary map          file 'on'
0 ; nefis/netcdf history file 'off'
0 ; nefis/netcdf map     file 'off'

#9           ; delimiter for the ninth group of input data
```

9.1 General

D-Water Quality is able to produce a number of output files. The contents of some of them can be steered with this input section. The time steps and / or time spans that are used for the output files are given in group 2 of the input file. There the start time, stop time and time step size of 3 types of files are given through:

◇ the monitoring file timer
◇ the map file timer
◇ the history file timer

These timers will be called mon-timer, map-timer and his-timer respectively There are more output files, but they all use one of these 3 timers.
This group of the input file steers the information that will be displayed in the files. By default all concentrations of modeled substances are part of the output in a file. The concentrations are expressed in $mass/m^3$ for the transported substances and in $mass/m^2$ for the passive substances. It is however also possible to add information that is computed by the water quality processes to the output files. Obviously useful extensions can be non-modeled derived quantities like Chlorophyll (the model models individual algae species in mgC/l) or Secchi depth. Especially in the set-up phase of a water quality model it is useful to also write output on intermediate computation results like the actual growth and mortality of the algae species, which is light and temperature dependent. This information is useful to check whether the model acts as expected. Once production simulations have to be conducted these entries
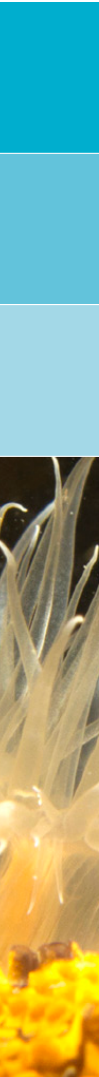
can be removed from the output files if there is no specific interest for them any more. The information that is added to the output files is added in exactly the same way as the modeled substances. In this way it is possible to make time series graphs, color contour graphs or 3D graphs of added variables as if they were modeled substances. Using the `PLCT` to select water quality processes and model inputs that will be available for external steering, it is also possible to view and select the quantities that can be added to the output files.

This is not the only location where the content of output files is determined:

◇ The keyword section of group 2 of the input file contains a number of directives to switch on the production of mass balance information. These directives may trigger the production of additional output to standard output files and the production of separate files with output of mass balance information. Although not directly steered by the input in this group, they will nevertheless be briefly described here.

◇ The monitoring area and monitoring transects section of group 2 of the input file allows the definition of other monitoring locations than just a simple cell. The definition of these areas and transects determines for which spatial locations additional output of time history data will be given. The output will be added to the monitoring file and to the history file.

◇ Group 10 of the input data deals with on-line statistics on variables. In this group it is possible to define a number of statistics that have to be computed during the simulation. The results of these statistics are saved either in the regular output files or in additional output files that are described in that section of the manual.

D-Water Quality used to produce two types of output files for history and map data: the plain binary files and the self-descriptive `NEFIS` files. Neither of these files contain any information on the shape of the grid. Deltares is now in a process to migrate the `NEFIS` output to `NetCDF` using the UGRID standard to describe the grid. It is now possible to replace the `NEFIS` map file by a `NetCDF` map file by specifying a file *WAQGEOM* file in group 3 of the input file.

9.2 Output files

D-Water Quality simulations have the following output files generated at run time:

1 the monitoring file (the `.mon` file)
  This is a user readable output file with:

  ◇ echo of simulation settings.
  ◇ diagnostic run-time messages.
  ◇ error messages as generated at run-time.
  ◇ global system mass balance.
  ◇ readable output of concentration values of state variables at the monitoring locations and additional variables at monitoring time steps.
  ◇ optional readable output of mass balances for monitoring areas. For multi cell monitoring areas it is essential to have the correct weighing option set for your mass balances variables. The options are ' ' (none), 'volume' and 'surf'. Option 'surf' has to be used for output per m^2, option 'volume' has to be used for output that is expressed per m^3.

  The monitoring file start, stop and step timings are given values in input group 3.
  The monitoring areas to write concentrations and generate balances for are defined in input group 3.

2 the grid-topology output file (the `.dmp` file)
  This is a user readable output file with concentration values of the selected substances printed in a user defined spatial pattern to reflect spatial phenomena.
  The grid-topology output file uses the start, stop and time step information of the map file.

3 the history output file (the `.his` file)
  This is a binary output file that is readable using the standard graphical post processing

software of D-Water Quality. It contains time series at selected monitoring areas and monitoring transects of concentration values and additional output variables. Also for the history file it is important to have the correct weighing option from 'volume' 'surf' and none (' ')

The history file start, stop and step timings are given values in input group 3.

The monitoring areas to write concentrations and additional output variables for are given in input group 3.

4 the map output file (the `.map` file)

This is a binary output file that is readable using the standard graphical post processing software of D-Water Quality. It contains complete fields of concentrations and additional output variables for the selected time steps.

The map start, stop and step timings are given values in input group 3.

5 the balances output file (the `-bal.his` file and the `-bal.prn` file)

This is a user readable output file and a binary output file that is readable using the standard graphical postprocessing software of D-Water Quality. They contain all mass balances terms of the selected monitoring areas for the model concentrations.

The balances output file uses the start, stop and time step information from the monitoring file.

6 the `NEFIS` or `NetCDF` history file (the `.hda` and `.hdf` files, or `_his.nc` file)

This file is equivalent with the binary history file and it uses the same timings. It is to be superseded by a `NetCDF` file version of the history file (see 3).

7 the `NEFIS` or `NetCDF` map file (the `.ada` and `.adf` files, or `_map.nc` file)

This file is equivalent with the binary map file and it uses the same timings. It is to be superseded by a `NetCDF` file version of the map file (see 3).

8 the statistical output map file (the `-stat.map` file)

This file has exactly the same structure as the binary map file. It starts to be processed at simulation start time, it stops at simulation stop time and uses the simulation time step. The file contains spatially distributed statistical data that is defined in the group 10 of the input file. The data is computed on the fly and may result in spatial fields of exceedence frequencies, time averaged values, standard deviations etc.

9 the statistical monitoring file (the `-stat.mon` file)

This is a user readable output file with statistical characteristics of the simulation that are not spatially distributed. It starts to be processed at simulation start time, it stops at simulation stop time and uses the simulation time step.

10 the restart file (the `.res` file and the `_res.map` file discussed in the group 8 input section)

It is to be expected that the writing of the `_res.map` file will be discontinued soon.

11 a `-timers.out` file that may assist in the analysis of computational performance of the simulation.

9.3 Additional output variables

By default the output files 1 - 4 from above list contain the concentrations of all modeled substances, either per m^3 for transported substances, or per m^2 for non-transported substances laying on the bed. It is however possible to add additional output variables to these four files. These additional output variables are defined in this ninth group of the input file. The input of this group consists of:

◇ an integer that can be:

-1 external input file

This is a remnant from the past and is equivalent with the `INCLUDE` directive. The name of an external file is expected after this '-1'.

1 continue with this input file

If the integer is missing and directly #9 follows, then this group is absent and default output processing (only modeled substances and their balances) will take place.

⬦ for each of four output file types:

- ▫ the monitoring file
- ▫ the grid topology output file
- ▫ the history file
- ▫ the map file

the following information is required that starts with an integer option number that can be:

0 no output is required for this file
1 default action is required for this file (output of modeled substances only)
2 the default output is required plus the items that are mentioned in the following listing
3 only the items that are mentioned in the following listing are required

The listing that should follow for integer values 2 and 3 consists of:

- ▫ the number of additional variables
- ▫ for each of the additional variables:

  - ○ the reserved ID of the variable (this is the ID that is also mentioned in the PLCT selection screen for output variables)
  - ○ ONLY for the monitoring and the history file, so the first and the third file:
    The string to indicate how to weigh the variable if it is aggregated for multiple cells. Valid strings are:

    - ▷ an empty string ' ', no specific weighing applied.
    - ▷ Volume to indicate that the aggregate should be weighed by volume. Advised for history files and transported substances.
    - ▷ Surf to indicate that the aggregate should be weighed by horizontal surface area of the grid cell. Advised for history files and passive substances laying on the bed.

⬦ for each of the four main binary output files an integer 1 when the file should be written or 0 when the file must not be written.

⬦ optionally, if you have specified the *UGRID* geometry file, the following keywords are available after the selection of the output files:

- ▫ NCFORMAT value – specifies the type of NetCDF file. Use a value of 4 for NetCDF4 and a value of 3 for NetCDF3. Currently NetCDF3 is the default.
- ▫ NCDEFLATE value – specifies the deflation (compression) level (NetCDF4 only). Valid values are 0 to 9. The higher the number the more the data will be compressed, using less disk space, but potentially requiring more processing time. The default level is 2.
- ▫ NCCHUNK value – specifies the so-called chunk size (NetCDF4 only). The chunk size is given in bytes. See the documentation on NetCDF4 for more information. Default: no chunking applied.
- ▫ NCSHUFFLE value – specifies whether shuffling will be applied or not (NetCDF4 only). By default shuffling is off. If the value given is "YES", shuffling is turned on.

Note that the effectiveness of these compression options depends on many factors and it is not possible to give rules of thumb for "best" use.

9.4 Finalization

This part of the input file is finalized with the #9 end of ninth data group indicator.

10 Statistical output

This is the tenth group in the input file. This input group may read like:

```
version 3 minor 28

period 'annual'
   suffix      'ann'
   start-time '1997/01/01-00:00:00'
   stop-time  'STOP'
end-period

period 'dry season'
   suffix      'dry'
   start-time '1997/01/01-00:00:00'
   stop-time  '1997/04/10-00:00:00'
end-period

output-operation 'STADAY'
   substance 'Salinity'
   suffix      ''
   time-parameter 'TINIT' 'START'
   time-parameter 'PERIOD' '0000/00/01-00:00:00'
end-output-operation

output-operation 'STAQTL'
   substance 'OXY'
   suffix      'p10'
   real-parameter 'CQLEV' 10
   real-parameter 'NOBUCK' 20
   real-parameter 'CLOBND' 0
   real-parameter 'CUPBND' 10
end-output-operation

output-operation 'STADSC'
   substance 'OXY'
   suffix     ' '
end-output-operation

output-operation 'STADPT'
   substance 'OXY'
   suffix     ' '
end-output-operation

output-operation 'STAGEO'
   substance 'EColi'
   suffix    'geo'
   real-parameter 'THRESH' 1
end-output-operation

 #10           ; delimiter for the tenth group of input data
```

10.1 General

It is always possible to conduct statistics with the output files of D-Water Quality simulations. You may read them and compute average values, standard deviations and percentiles of the concentrations that you read. Besides the fact that this will necessitate you to write computer programs yourself with all associated inconveniences, it may also be that the data in the files are too sparse to conduct sensible statistics with. If you want to identify spatial patterns of average values, standard deviations and excess percentiles, then the only suitable dataset is the binary `.map` file. One complete record in the map file is already as large as the number of substances and additional variables times the number of computational cells. This may be
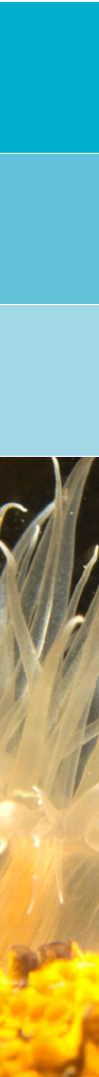
a large amount and you may feel forced to limit the frequency of writing `.map` files. But then you also limit the frequency of available data for statistical analysis.

To support you somewhat with your statistical analysis it is possible to let D-Water Quality compute summary statistics on the fly, using every time step of the simulation, also those that are not written to file. Input group 10 contains the input needed to use this facility. The input has two distinct parts:

◇ Definition of time intervals for statistical evaluations
◇ Definition of the statistics wanted, together with for some of them the required and optional coefficients

The statistical input may be preceded by the definition of a version number and a version sub-number after the `VERSION` and the `MINOR` keywords respectively.

10.2   Definition of time intervals

The definition of time intervalsStatistics!intervals has to follow the following rules:

◇ They are enclosed by the `PERIOD` and the `END-PERIOD` keywords
◇ Any number of time intervals may be defined, but you must be aware that all intervals are used by all the statistics that work on intervals.
◇ Intervals have a name that is specified immediately after the `PERIOD` keyword.
◇ Intervals may have a suffix or abbreviation. This suffix is essential and should be unique if you have multiple intervals. It is added to the name of the output variable to allow for identification. The suffix should be brief, because otherwise the name of the output variable will run out of space. The suffix is specified by the keyword `SUFFIX` followed by the suffix itself.
◇ Intervals may have a start time string following the keyword `START-TIME`. The default value for the start time is the start-of-simulation. This default value can also be specified by the user stating that the start time string is `START`.
◇ Intervals may have a stop time string following the keyword `STOP-TIME`. The default value for the stop time is end-of-simulation. This default value can also be specified by the user stating that the stop time string is `STOP`.

All specified intervals are applied for all the statistical procedures that work on intervals.

10.3   Supported statistical procedures

The following statistical evaluations are supported:

◇ Periodic averages
Invoked with the keyword `STADAY`
The result is a time function that is updated at the end of the period. It is saved in the D-Water Quality binary and `NEFIS` map and history output files.
This statistic requires two `TIME-PARAMETER` strings:

▫ a `TINIT` with default value `START`
▫ a `PERIOD` for the average.

These statistics are evaluated for the complete modelling period since `TINIT`.
◇ Depth average, minimum and maximum
Invoked with the keyword `STADPT`
The resulting three statistics are added to the D-Water Quality binary and `NEFIS` map and history output files and are identical in these files for all layers.
These statistics are evaluated for the complete modelling period.

No further input is required.

◇ Maximum, Minimum, Mean and Standard deviation values
Invoked with the keyword STADSC
The resulting four statistics per period are written to a separate -stat.map and -stat.mon file.
These statistics are evaluated for all defined periods in this input group.
No further input is required.

◇ Excess frequencies and Geometric means with and without threshold value
Invoked with the keyword STAGEO
The resulting three statistics per period are written to a separate -stat.map and -stat.mon file.
These statistics are evaluated for all defined periods in this input group.
The statistic requires a REAL-PARAMETER called THRESH, a threshold below which the data are omitted.

◇ Excess frequencies and Average during excess
Invoked with the keyword STAPRC.
The resulting two statistics are written to a separate -stat.map and -stat.mon file.
These statistics are evaluated for all defined periods in this input group.
The statistic requires two parameters:

   □ a REAL-PARAMETER called CCRIT, the excess threshold.
   □ a LOGICAL-PARAMETER called ABOVE that can have value 'yes' if frequency and average above threshold should be computed and value 'no' if frequency and average below threshold should be computed.

◇ Quantiles
Invoked with the keyword STAQTL
The resulting quantile per period is written to a separate -stat.mon file.
These statistic is evaluated for all defined periods in this input group.
This statistic requires four REAL-PARAMETERS:

   □ a CLOBND followed by the expected lower bound value of the data.
   □ a CUPBND followed by the expected upper bound value of the data.
   □ a NOBUCK followed by the number of buckets or baskets to use between the bounds.
   □ a CQLEV followed by the quantile level whose value is sought.

10.4 Definition of statistical procedures

The definition of statistical procedures has to follow the following rules:

◇ They are enclosed by the OUTPUT-OPERATION and the END-OUTPUT-OPERATION keywords.
◇ Any number of statistical procedures may be defined.
◇ Statistical procedures have an ID that is one of STADAY; STADPT; STADSC; STAGEO; STAPRC and STAQTL.
◇ Statistical procedures have a substance ID where they work on. The substance ID is defined after the keyword SUBSTANCE.
◇ Statistical procedures may have a suffix or abbreviation. This suffix is essential and should be unique if you have multiple occurrences of the substances in the statistical procedures, because it is added to the name of the output variable to allow for identification. The suffix should be brief, because otherwise the name of the output variable will run out of space. The suffix is specified by the keyword SUFFIX followed by the suffix itself.
◇ Statistical procedures may have steering variables. These variables may be of the type REAL-PARAMETER; TIME-PARAMETER or LOGICAL-PARAMETER. The type is followed by the reserved parameter name (see the section on supported statistical procedures) and by the value of the parameter.

10.5 Statistical output files

The thus computed statistical information is:

◇ Added to the D-Water Quality binary and Nefis map and history file for

▫ periodic averages `STADAY`.
They will have the 5 letter prefix `TAVG_`.
▫ depth averages `STADPT`.
They will have the 7 letter prefix `DPTAVG_`, `DPTMIN_`, and `DPMAX_`

◇ Written to a separate D-Water Quality binary and Nefis `-stat` map file and the `ASCII` monitoring file for

▫ Maximum, Minimum, Mean and Standard deviation `STADSC`.
They will have the prefix `MIN_`, `MAX_`, `MEAN_` and `STDEV_`.
▫ Excess frequencies and Geometric means with and without threshold value `STAGEO`.
They will have the prefix `T_GEO_`, `GEO_`, `ALL_GEO_` respectively.
▫ Excess frequencies and Average during excess `STAPRC`.
They have *NO* prefix and `CMN_` respectively as prefix.

◇ Written to a separate D-Water Quality `ASCII` monitoring file for

▫ Quantiles `STAQTL`.
They have *NO* prefix.

10.6 Finalization

This part of the input file is finalized with the `#10` end of tenth data group indicator.

11 Annexes

11.1 Time tokens

You often need to specify times to D-Water Quality:

◇ for the start and stop time of the time integration.
◇ for the start and stop time of writing certain output files.
◇ for the times of breakpoints in a specified time series for:

□ for time series of hydrodynamic inputs if not generated by a hydrodynamic model.
□ for time series of concentrations at open boundaries.
□ for time series of loads of substances through rivers and outfalls.
□ for time series of process steering functions or segment functions.

◇ for the start and stop times of run-time statistics evaluation.

You may also need to provide time step sizes to D-Water Quality:

◇ for the integration procedure.
◇ for the writing of output files.
◇ to specify time lags or time delays.

You can provide times to D-Water Quality in 2 ways:

◇ as an integer:
This integer is interpreted according to the specifications in group 1 as:

□ The system time (generally in seconds)
□ According to the `DDHHMMSS` format
□ According to the `YYDDDHH` format

The disadvantage of this procedure is that a year will always have 365 days.
The advantage of this procedure is that it is independend of the actual calendar period of your model simulation and allow the input to be reused for other cases, irrespective of the actual calendar dates of the simulation.
This integer input is the only way to provide time step information to D-Water Quality.
◇ as a string:
This string should obey exact formatting rules and looks like:

$$2010/07/31-12:00:00$$

This format is only allowed if the Calendar offset in the 4th title string in group 1 is specified. D-Water Quality will convert such a title string in relative system times using the following procedure:

□ The time string is converted to a so-called *Julian date*
□ The *Julian date* of the Calendar offset is subtracted from this value
□ The difference is converted to relative system time units

The important advantage of this procedure is that months and years have their correct amounts of days and that you can input real dates.

If other input than an integer or a valid calendar time string is provided, several things can happen:

◇ If a real value is encountered then either:

□ A context dependent path is chosen to interpret the real value in a sensible way, like a

concentration or a coefficient if the local context allows such an item to appear at that location in the file.

□ An error is produced stating that a real value was found whereas an integer or a string was expected. This happens if a real value cannot appear according to the local context of the file.

◇ If a string is encountered that does not equal to a valid calendar time string, then either:

□ A context dependent path is chosen to interpret the string in a sensible way, like the name / ID of a substance or of a coefficient if the local context allows such an item to appear at that location in the file.

□ An error is produced stating that the string read was not a valid calendar time string. This happens if a string value cannot appear according to the local context of the file.

Be aware that:

◇ the system time values are stored in a 32-bits signed integer and can thus only run from -68 years to +68 years.

◇ the DDHHMMSS format has a highest value of 2^{31} = 2147483648 or 5 years of 365 days and 322 days, 48 hours, 36 minutes and 48 seconds.

◇ the YYDDDHH format is only limited by the -68 to +68 years time window.

11.2 Hydrodynamic input

◇ The input of hydrodynamic data for all segments (the volumes) or for all exchange surfaces (the areas, flows, velocities and dispersions) starts with an integer option number:

-4 A so called MULTIPLE_HYD file will be used.

□ optionally the keywords UNFORMATTED and BIG_ENDIAN are allowed to indicate the specific structure of the binary files that will be used in this description.

□ an integer indicating the number of lines that should be read from the multiple hyd file.

□ an integer interpolation option in time, between the records in the files with 1 is no interpolation and 2 is linear interpolation

□ an identification string for this type of data like 'volumes-file', 'areas-file', 'flows-file' or 'vert-diffusion-file'. This string should correspond exactly with the file that is to be used from the files that are listed in the .hyd file. Also for the salinity, temperature chezy coefficients, shear stresses or suspended sediments as computed by the hydrodynamic model it is possible to follow this procedure by mentioning the corresponding keyword from the .hyd file.

□ the name of the multiple hyd file to be used.

-2 A binary external file will be used that will be interpolated between its records. This option number can optionally be followed by the keywords UNFORMATTED and BIG_ENDIAN and should be followed by the file name to be used.

-1 This is the same as the INCLUDE directive (its 'old-style' predecessor) that should be followed by and ASCII input file name to switch input processing to.

0 A binary external file will be used with one time step per record. This file will not be interpolated. This option number can optionally be followed by the keywords UNFORMATTED and BIG_ENDIAN and should be followed by the file name to be used.

1 ASCII input will follow in this file.

Any other option number will result in an error message. If the option number was zero, then the input is done. The information will be read from the specified file. Input is also done if the option number was -4 or -2 and the subject of this reading was not dispersions.

◇ If dispersions are to be read, the following is required:

□ three real values as scale factors for the dispersions in the three directions.

□ three real values that contain the yet unscaled values of the dispersions in the three directions.

◇ `ASCII` input if the first option was -1 or 1
This input starts with a data option number:

1 Information is constant and input will be provided without defaults:
For all of the three directions that have non-zero number of exchanges the following should be provided:

□ A scale factor for this direction.

□ A matrix of data with as columns (fastest running index) the number of values to be read per volume or exchange with for each of the number of volumes or exchanges in this direction a row with the unscaled values.

The scale factor is applied to all specified values in its direction.

2 Values are constant and input will be provided using default values:
For all of the three directions that have non-zero number of exchanges the following should be provided:

□ A scale factor for this direction.

□ For each of the required values per volume or exchange, an unscaled default value.

□ A number of overridings (exceptions to the default settings) plus that many sets of:

○ An exchange number that should be overriden with the exceptional values.

○ For each of the required values per volume or exchange an unscaled exceptional value.

The scale factor is applied to all specified default values and exceptional values in its direction.

3 Information comes as time functions:
Now for all volumes or exchanges time functions are specified through `ASCII` input for all required values. This happens using the standard 'old-style' feature for input processing of time functions that is hardly used any more. The input is structured in input blocks that all start with an integer option number:

1 Information in this block is given at breakpoints as a block function (no linear interpolation)

□ an integer giving the number of items (exchange numbers or segment numbers for hydrodynamics) that will be contained in this input block.

□ the item numbers of the items that are contained in this input block.

□ an integer giving the number of breakpoints

□ a real value for each required scale value. For hydrodynamic data generally 1 scale value is required per direction in the grid (so certainly also per input block).

□ then for each breakpoint:

○ either an absolute time string, or a time integer indicating the time stamp of this breakpoint.

○ a matrix with values per breakpoint.
The matrix has 1 column for the reading of volumes, areas and flows. It has 2 columns for the reading of the 'from' and 'to' lengths and it has as much columns as there are additional velocity and dispersion arrays specified for the reading of additional velocities and dispersions.
The rows in the matrix are the items that are contained in this input block.

2 Information in this block is given at breakpoints, interpolation will be linear.

The input structure and type of input information for this option is exactly equal to that of option 1.

3 Information in this block is given as a set of harmonic functions.

▫ an integer giving the number of items (exchange numbers or segment numbers for hydrodynamics) that will be contained in this input block.
▫ the item numbers of the items that are contained in this input block.
▫ an integer giving the number of harmonic components that will be read, exclusive of the zeroth component, the average value of the series.
▫ for each item in this block the average value of the harmonic series.
▫ for each harmonic component:

○ an integer period of the harmonic component (in units of the system clock).
○ a real value giving the phase of this component.
This real value can be between -0.5 and +0.5 with no phase shift at value 0.0. It can equally well be between 0.0 and 1.0 with no phase shift at values 0.0 and 1.0. This does not matter because the harmonic function is cyclic and the phase shift is expressed as fraction of the period of the component.
○ a matrix with amplitude values of the component.
The matrix has 1 column for the reading of volumes, areas and flows. It has 2 columns for the reading of the 'from' and 'to' lengths and it has as many columns as there are additional velocity and dispersion arrays specified for the reading of additional velocities and dispersions.
The rows in the matrix are the items that are contained in this input block.

4 Information in this block is given as a Fourier series.

▫ an integer giving the number of items (exchange numbers or segment numbers for hydrodynamics) that will be contained in this input block.
▫ the item numbers of the items that are contained in this input block.
▫ an integer giving the number of Fourier components that will be read, exclusive of the zeroth component, the average value of the series.
▫ an integer giving the base period, the period of the first Fourier component
▫ for each item in this block the average value of the Fourier series
▫ for each Fourier component:

○ a real value giving the phase of this component.
This real value can be between -0.5 and +0.5 with no phase shift at value 0.0. It can equally well be between 0.0 and 1.0 with no phase shift at values 0.0 and 1.0. This does not matter because the Fourier function is cyclic and the phase shift is expressed as fraction of the period of the component.
○ a matrix with amplitude values of the component.
The matrix has 1 column for the reading of volumes, areas and flows. It has 2 columns for the reading of the 'from' and 'to' lengths and it has as much columns as there are additional velocity and dispersion arrays specified for the reading of additional velocities and dispersions.
The rows in the matrix are the items that are contained in this input block.

11.3 Multiple hyd file

It can be convenient to compose a hydrodynamic scenario from single simulations. One could e.g. have a simulation for a typical dry monsoon sprin-neap tide period and a wet monsoon spring-neap tide period. D-Water Quality rewinds the hydrodynamic dataset if the simulation lasts longer than the dataset. At some moment the dry season may shift into a wet season and then one would want D-Water Quality to shift to a different input file. For this reason the *multiple hyd* file feature was developed. It allows the construction of a hydrodynamic scenario by stating from which simulation time which hydrodynamic dataset has to be used with which time delay, to control the phasing in tide and spring-neap cycle. The set of files that form together a hydrodynamic dataset are generally described in an ASCII `.hyd` file like is produced by Delft3D-FLOW or Telemac. This means that a *multiple hyd* file just needs to refer to these `.hyd` files. An example is in a real-life marine application:

```
1.0 1996/12/02-05:00:00 1997/05/01-15:00:00 1996/12/02-07:00:00 'com-92d.hyd'
0.5 1997/05/01-15:00:00 1997/05/31-17:00:00 1996/12/02-05:00:00 'com-92d.hyd'
0.5 1997/05/01-15:00:00 1997/05/31-17:00:00 1996/05/31-17:00:00 'com-92w.hyd'
1.0 1997/05/31-17:00:00 1997/07/30-21:00:00 1996/05/31-17:00:00 'com-92w.hyd'
0.5 1997/07/30-21:00:00 1997/08/29-23:00:00 1996/12/02-05:00:00 'com-92d.hyd'
0.5 1997/07/30-21:00:00 1997/08/29-23:00:00 1996/05/31-17:00:00 'com-92w.hyd'
1.0 1997/08/29-23:00:00 1998/01/01-00:00:00 1996/12/02-05:00:00 'com-92d.hyd'
```

The example says that:

◇ With weight factor 1.0

- □ From 1996/12/02-05:00:00 to 1997/05/01-15:00:00
- □ Files from 'com-92d.hyd' (dry season) are used
- □ Starting from the time in the file of 1996/12/02-07:00:00
  In the first line of this example the starting point in the file is 2 hours later than the start of the file. This starting point in the file gives opportunity to adjust the periodicity such that e.g. a high water of the preceding period connects to a high water of the following period. If the files are rewound during a period, then they are rewound towards the start time of the file again.

◇ During a 30 days + 2 hour transition period in May, 0.5 * the dry season files '92d' and 0.5 * the wet season files '92w' are used.
◇ During June and July the wet season files only are used.
◇ During August again a transition period of both type of files with 0.5 / 0.5 weight factors is used.
◇ From late August to the end of the year the dry season files only are used again.

There are two special weight factors available:

-1.0 these files will linearly diminish in weight from 1.0 to 0.0 during the period.
 0.0 these files will linearly increase in weight from 0.0 to 1.0 during the period.

The reference to the *multiple hyd* file starts with 2 integers in the calling input file:

◇ The number of lines to be used in the *multiple hyd* file (would be 7 in our example).
◇ The interpolation option that can be:

- 0 for block wise interpolation in time (flows and areas).
- 1 for linear interpolation in time (volumes).
- 2 for linear interpolation of the logarithms of the file values block wise in time (vertical diffusions).

    3 for linear interpolation of the logarithms of the file values both between files and in time.

A number of remarks should be made:

◇ It is the responsability of the user to figure out that the water level at the end of a specified period, more or less is in concert with the water level at the start of the next period. This can be done by a judicious choice of the start time in the mentioned files for the next period.
◇ Within each period, the files are rewound and reused with the same scale value if end-of-file is reached during the period.
◇ At the end of the period the description for the next period is used.
◇ Should the simulation extend beyond the specification periods in the *multiple hyd* file, then the whole *multiple hyd* file is rewound and executed again.
◇ For a check it is strongly advised to output at several locations the time series of water levels for inspection.
◇ Both if rewound and if specifications change, the presence of the CLOSE_ERR constant determines whether the concentration will show a (small) jump or whether the mass will do.

11.4   Binary file that are directly read by D-Water Quality

Binary filesare very efficient to read. That is why D-Water Quality allows the input from bulky binary files that are written e.g. by the hydrodynamic model that produced flow fields. Many scientific software is written in a flavor of the FORTRAN programming language. This makes it very likely that your binary input files for D-Water Quality are written by FORTRAN. The ANSI standard for that language however does not support binary files. FORTRAN supports unformatted files. These are also very efficient to read but they have record information included in the file. This record information is compiler specific so although a standard exists for the unformatted file in the FORTRAN language, the contents of that file may vary per implementation. If you are using the same compiler for your hydrodynamic program as was used for our D-Water Quality source code, then there are not so much problems. Before mentioning the name of your binary file in the input file you just give the keyword UNFORMATTED and D-Water Quality will open and read the file as an unformatted file. If you are using a very recent compiler, you may open and write your hydrodynamic files with the ACCESS = 'STREAM' option in your source code. That is more or less equivalent with the binary files that D-Water Quality is reading normally.

Binary files consist of bit patterns indicating the numbers rather than readable characters. There are several bit patterns around to write integer and real numbers. D-Water Quality is using the IEEE standard with 'little endian' layout of the bytes. That is the common layout on PC type of processors. Main frames and workstations may be equiped with processors that use the 'big endian' layout of bytes. If you are facing those files you may also use the keyword BIG_ENDIAN before you specify the name of the binary file to be read by D-Water Quality.

In the following a documentation of the contents of the binary files that are directly read by D-Water Quality is given. This specification also mentions the batches of data that D-Water Quality reads from them separately. This would normally not be of importance. As long as you have written your data in the same order in the binary file, then it does not matter in what chunks D-Water Quality reads them. This is however not the case for unformatted files. They contain record information and the chunks used for reading need to be exactly identical to the chunks used for writing. To support you with that the specification contains the reading procedure.

The table 11.2 gives a list of binary files that are read directly by D-Water Quality. Each ● indicates a new record for unformatted files. The matrices (nn, mm) indicate $nn*mm$ values with the nn index running fastest. The capital amounts refer to the dimensions mentioned in the corresponding sections of theis manual:

Table 11.1: Dimensions mentioned in table 11.2

Variable	Legenda
NX, NY	First and second dimensions of the plot grid
NOSEG	Number of computational cells
NMAX, MMAX	First and second dimension of the hydrodynamic grid
NOSEGL	Number of active cells in one layer
NOLAY	Number of layers
NOQ1, NOQ2, NOQ3	Number of exchanges in
NOQT	Sum of NOQ1, NOQ2, NOQ3
NODISP	Number of additional dispersion arrays
NOVELO	Number of additional velocity arrays
NOPARAM	Number of parameters that are defined for this file
NSEGFUN	Number of segment functions that are defined for this file **Note:** the matrix is transposed for this file

Table 11.2: Documentation of the binary input files that can be read directly by D-Water Quality

File	Records
plot grid segment properties	● `NOSEG` integer*4, one for each segment
segment volumes	● 'time' integer*4, `NOSEG` real*4 volumes ● same for next time step(s) ● · · ·
regular grid	● 7 integer*4, `NMAX`, `MMAX`, `NOSEGL`, `NOLAY`, `NOQ1`, `NOQ2`, `NOQ3` ● (`NMAX,MMAX`) matrix of integer*4 values with active grid layout
exchange pointer	● 4 integer*4 `ifrom, ito, ifrom-1, ito+1`

File	Records
	• the same for all other `NOQT = NOQ1+NOQ2+NOQ3` exchanges • · · ·
dispersions	• 'time' integer*4, `(NODISP,NOQT)` matrix of real*4 values • same for next time step(s) • · · ·
flows	• 'time' integer*4, `NOQT` real*4 values • same for next time step(s) • · · ·
exchange areas	• 'time' integer*4, `NOQT` real*4 values • same for next time step(s) • · · ·
velocities	• 'time' integer*4, `(NOVELO,NOQT)` matrix of real*4 values • same for next time step(s) • · · ·
exchange lengths	• 'time' integer*4, `(2,NOQT)` matrix of real*4 values • (1,:) = dx for left/1st cell to interface • (2,:) = dx for interface to right/2nd cell • same for next time step(s) • · · ·
parameters	• `(NOPARAM,NOSEG)` matrix of real*4 values
segment functions	• 'time' integer*4, `(NOSEG,NSEGFUN)` matrix of real*4 values • same for next time step(s) • · · ·

Deltares, 2016. "BIBTEX key with no entry, needed if no citations are made in the document."

Index

Photo by: Mathilde Matthijsse, www.zeelandonderwater.nl

Deltares systems