Water quality and aquatic ecology modelling suite

D-Water Quality

Deltares system

DRAFT

NESTWQ

User Manual

Deltares

D-WAQ NESTWQ

Offline nesting of water quality models

User Manual

D-Water Quality

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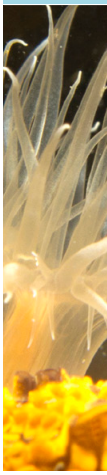

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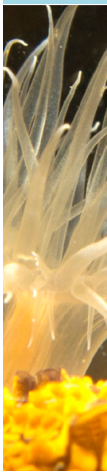


1 A guide to this manual

1.1 Introduction

This User Manual concerns the offline water quality nesting module, D-WAQ NESTWQ, of the Delft3D software suite. To make this manual more accessible we will briefly describe the contents of each chapter and appendix.

If this is your first time to start working with D-WAQ NESTWQ we suggest you to read and practice the getting started of Chapter 3 and the tutorial of Chapter 5. These chapters explain the user input and guide you through the definition of your first nested simulation.

Chapter 2: Introduction to D-WAQ NESTWQ, provides specifications of D-WAQ NESTWQ, such as the areas of applications, the functionality provided and an overview of the system.

Chapter 3: Getting started, explains the use of the overall menu program, which gives access to all Delft3D modules and to the pre- and post-processing tools. D-WAQ NESTWQ being one of them as part of the WAQ module.

Chapter 4: Input and output, provides detailed information on the parameters in the input file and the output files from D-WAQ NESTWQ.

Chapter 5: Tutorial, emphasis at giving you some first hands-on experience in using the D-WAQ NESTWQ tool.

Chapter 6: Limitations, warnings and errors, discusses the underlying assumptions and warnings and errors that might occur.

Chapter 7: Description files, explains in detail the contents of input and output files.

Chapter 8: Theoretical background, provides information about boundary segments, nest segments and weights.

References, provides a list of related Delft3D modules and background information.

1.2 Manual version and revisions

A manual applies to a certain release of the related numerical program. This manual applies to D-WAQ NESTWQ 1 version 2.00.02 and D-WAQ NESTWQ 2 version 2.00.03.

1.3 Typographical conventions

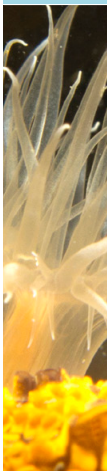
Throughout this manual, the following conventions in text formats help you to distinguish between different types of text elements.

Example	Description
Module **Project**	Title of a window or a sub-window are in given in **bold**. Sub-windows are displayed in the **Module** window and cannot be moved. Windows can be moved independently from the **Module** window, such as the **Visualisation Area** window.

Example	Description
Save	Item from a menu, title of a push button or the name of a user interface input field. Upon selecting this item (click or in some cases double click with the left mouse button on it) a related action will be executed; in most cases it will result in displaying some other (sub-)window. In case of an input field you are supposed to enter input data of the required format and in the required domain.
<\tutorial\wave\swan-curvi> <siu.mdw>	Directory names, filenames, and path names are expressed between angle brackets, <>. For Linux environments a forward slash (/) is used instead of the backward slash (\) for Windows environments.
“27 08 1999”	Data to be typed by you into the input fields are displayed between double quotes. Selections of menu items, option boxes etc. are described as such: for instance ‘select *Save* and go to the next window’.
`delft3d-menu`	Commands to be typed by you are given in the font Courier New, 10 points.
➢	In this User manual, user actions are indicated with this arrow.
[m s^{-1}] [–]	Units are given between square brackets when used next to the formulae. Leaving them out might result in misinterpretation. Most units will be in SI notation. [m AD] stands for ’meter Above Datum’, which denotes a level relative to the vertical reference system in the model.

2 Introduction to D-WAQ NESTWQ

The transfer of data from an encompassing or 'overall' numerical model to an embedded or 'nested' numerical model is called nesting. In general the overall model has a coarse resolution of grid cells, whereas the nested model has a higher resolution. At the boundary locations of the nested model the results from the overall model are required as boundary conditions for the nested model. The boundary conditions can be water levels, currents, fluxes or discharges in case of hydrodynamic models, and water quality parameters in case of water quality models.



2.1 System name and subsystems

The procedure of nesting through concentrations between D-Water Quality (Deltares, 2024a) (or Deltares (2024b)) models is performed by the system NESTWQ. In this procedure two steps can be distinguished which are handled by separate subsystems:

- ◇ D-WAQ NESTWQ 1, for the determination of nest segments and nest weights in the overall model. The concentrations at these segments are used by the next subsystem.
- ◇ D-WAQ NESTWQ 2, for the generation of boundary conditions for the boundary segments in the nested model from the results at the nest segments in the overall model.

2.2 Functionality

The functionality of the subsystem D-WAQ NESTWQ 1 is:

- ◇ determine for each boundary segment in the nested model which nest segments in the overall model are required for the nesting of results to these boundary segments
- ◇ determine for each nest segment the weight factors for the interpolation from the surrounding nest segments to the boundary segment in the nested model

The functionality of the subsystem D-WAQ NESTWQ 2 is:

- ◇ interpolate the concentration time-series from the nest segments in the overall model to boundary conditions for the boundary segments in the nested model
- ◇ average these boundary conditions in case of aggregated boundary segments in the nested model
- ◇ generate a D-Water Quality boundary conditions file for the nested model

2.3 Overview subsystems

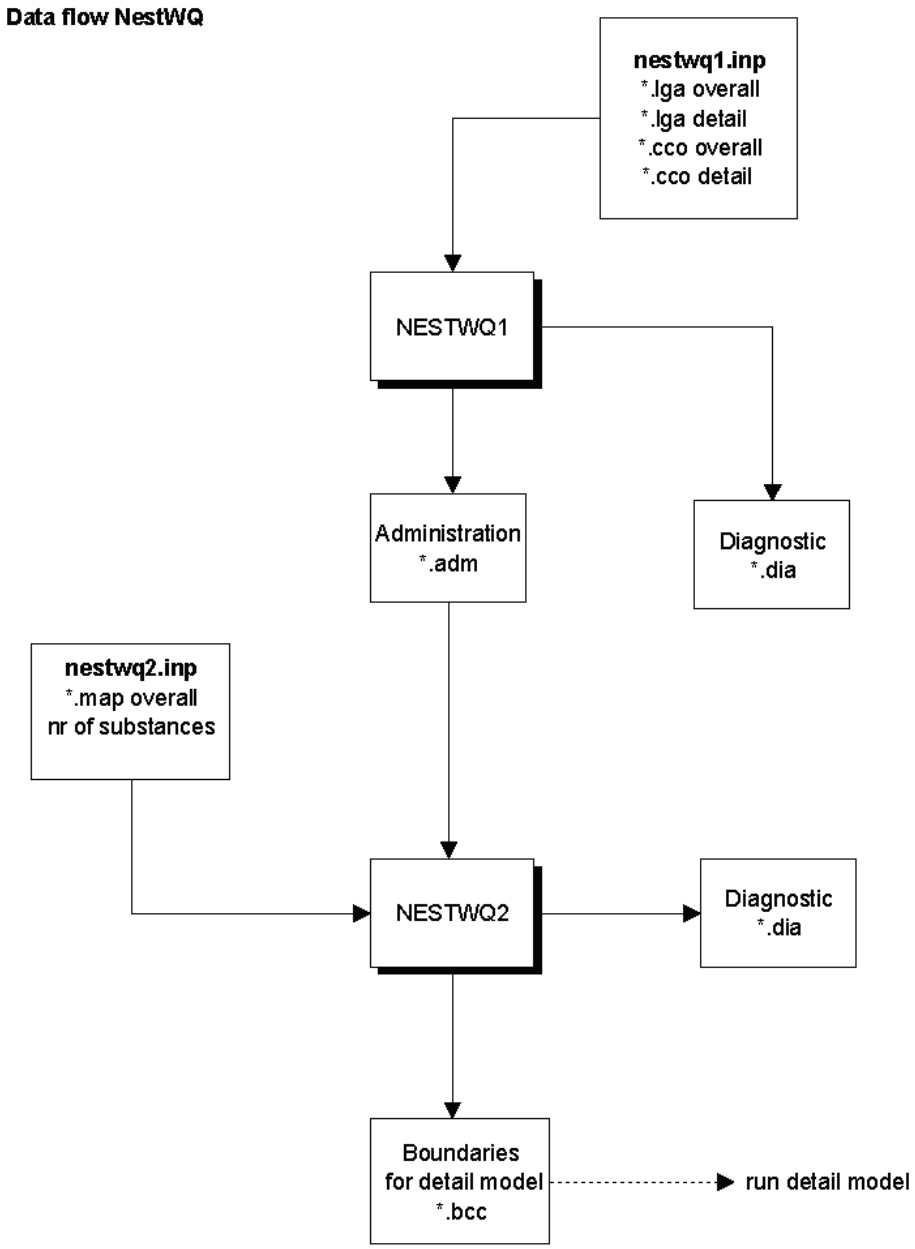


Figure 2.1: *Data flow diagram of D-WAQ NESTWQ*

3 Getting started

3.1 Starting Delft3D

To start Delft3D:

- ◇ On an MS Windows platform: select Delft3D in the Applications menu or click on the Delft3D icon on the desktop.
- ◇ On Linux and UNIX machines: type Delft3D-MENU on the command line.

Next the title window of Delft3D is displayed, Figure 3.1:

After a short while the main window of the Delft3D-MENU appears, Figure 3-2.

Whether or not you may use specific Delft3D modules and features depends on the license file you have. For now, only concentrate on exiting Delft3D-MENU, hence:

- ◇ Select *Exit*.

The window will be closed and you are back in the Windows Desk Top screen for PCs or on the command line for Linux and UNIX workstations.

Remark:

- ◇ In this and the following chapters several windows are shown to illustrate the presentation of Delft3D-MENU and D-WAQ NESTWQ. These windows are grabbed from the PC-platform. For Linux and UNIX workstations the content of the windows is the same, but the colours may be different. On the PC-platform you can set your preferred colours by using the Display Properties.

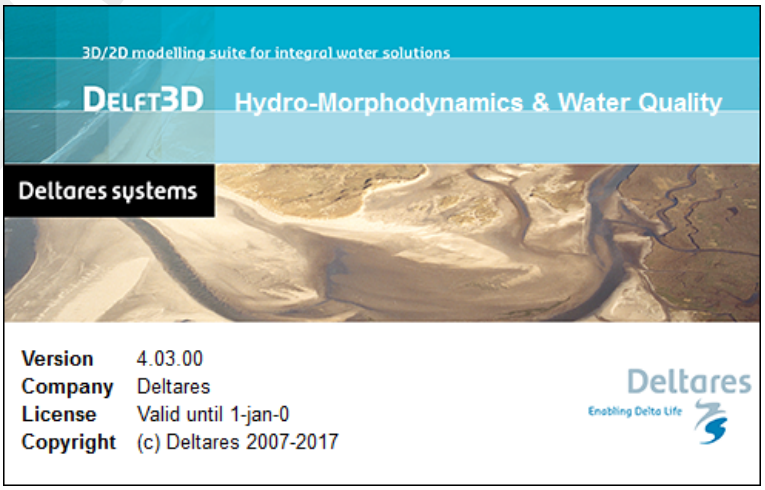


Figure 3.1: *Title window of Delft3D*

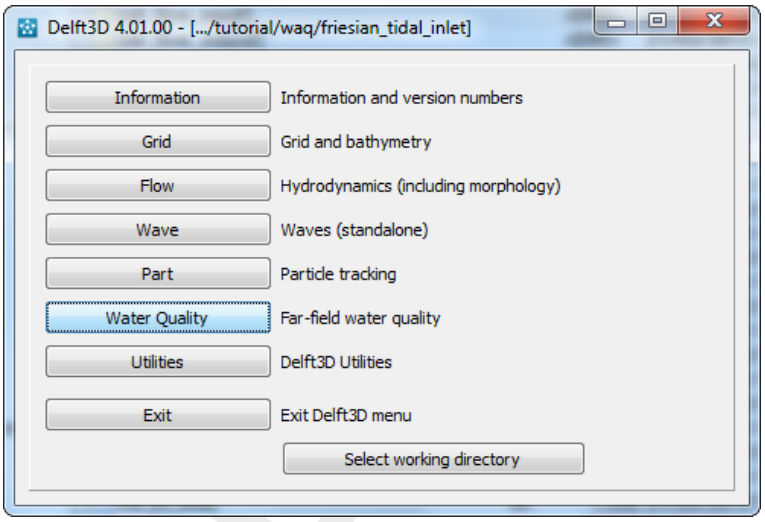


Figure 3.2: *Main window Delft3D-MENU*

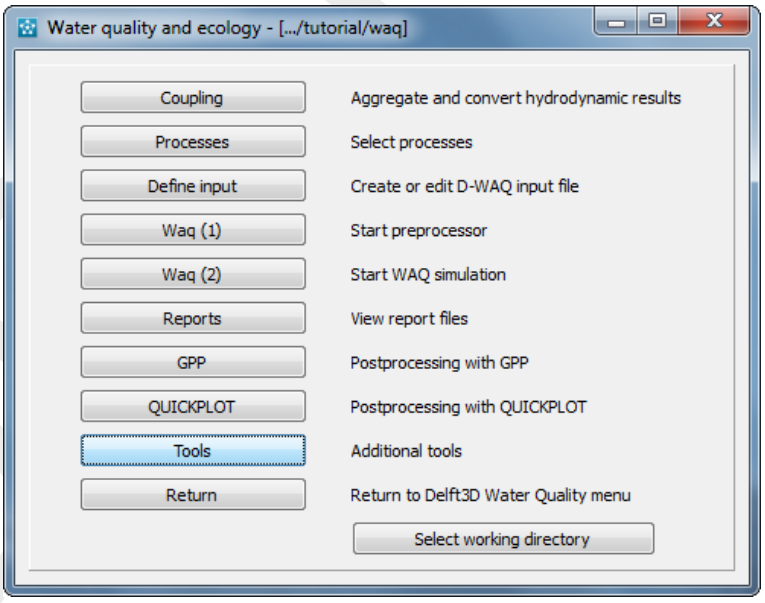


Figure 3.3: *Selection window for* ***Water Quality and ecology***

3.2 Getting into D-WAQ NESTWQ

To continue restart the menu program as indicated above. To access the nesting tool between an overall water quality model and a detailed water quality model, select the far-field water quality module.

◇ Select *Water Quality* in the main window, see Figure 3.2.

The nesting functionality is exactly the same for all water quality modules, therefore:

The selection window for **Water quality (WAQ)** is displayed (Figure 3.3), in which you can convert and/or aggregate hydrodynamic results, prepare a substance file using the Process Library Configuration Tool, prepare a water quality input file, run the pre-processor, execute a computation, inspect the report files with information on the execution, visualise the results, and access additional tools.

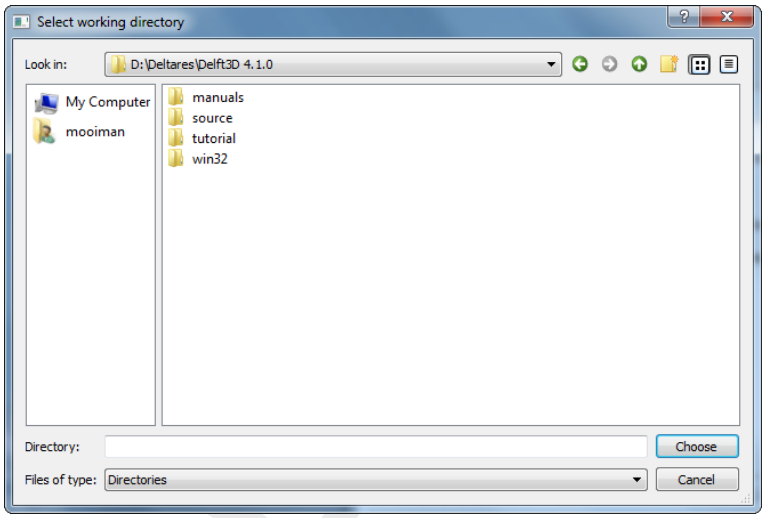


***Figure 3.4: Select working directory** window*

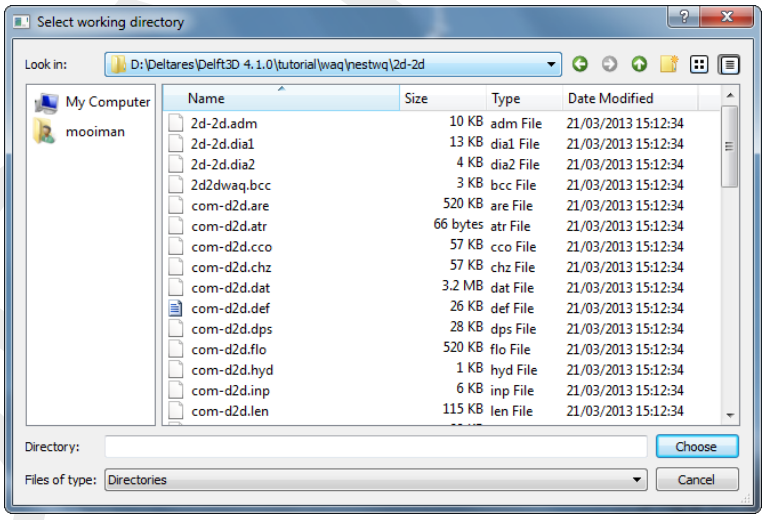


***Figure 3.5: Select working directory** window to set the working directory to <waq\nestwq\2d-2d>*

Before continuing with any of the selections of this **Water quality (WAQ)** window, you must select the directory in which you are going to nest water quality results:

◇ Click the *Select working directory* button.

Next the **Select changing directory** window, Figure 3.4, is displayed (your current directory may differ, depending on the location of your Delft3D installation).

◇ Browse to and enter the <Tutorial> sub-directory of your Delft3D Home-directory.
◇ Enter the <waq> directory. Next the <nestwq> sub-directory.
◇ Enter the <2d-2d> sub-directory and close the **Select working directory** window by clicking *OK*, see Figure 3.5.

Next the **Water quality (WAQ)** window is re-displayed, but now the changed current working directory is displayed in the title bar, see Figure 3.6.

Figure 3.6: *Current working directory*

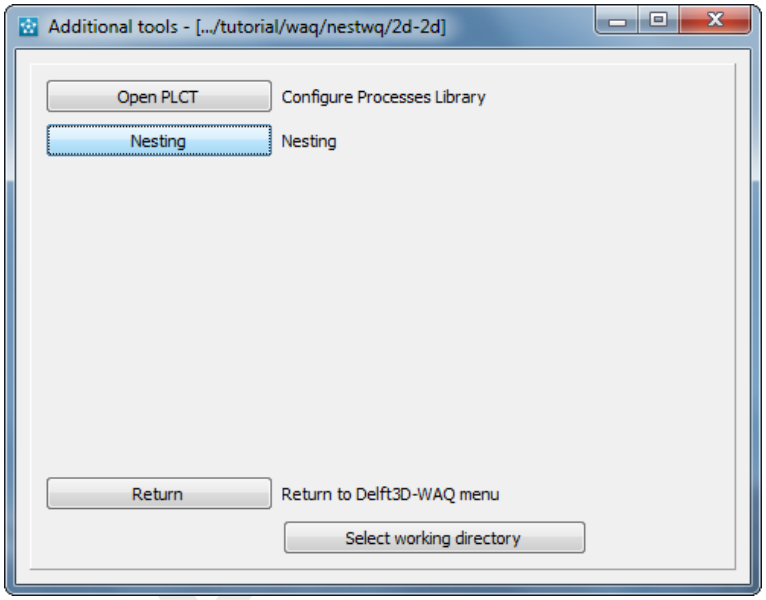


Figure 3.7: *Selection window for* ***Additional tools***

The nesting tools are part of the Additional tools, hence:

◇ Click on *Tools*.

The **Additional tools** window, Figure 3.7, contains the supporting programs to configure your own Processes Library and to nest water quality models.

◇ Click on *Nesting* to show the various steps in the nesting of water quality models, see Figure 3.8.

◇ Click on *Nest Input (1)*.

The input file for NESTWQ1 is opened, see Figure 3.9.

◇ Select *File – Exit*, to close the input file.
◇ Select *Return*, to close the **Additional tools** window.
◇ Select *Return*, and *Return* twice again, to enter the main window of Delft3D-MENU.
◇ Click *Exit*.

The window is closed and the control is returned to the desk top or the command line.

3.3 Exploring some menu options

To guide you through some menu options please follow the example in Chapter5, Tutorial.

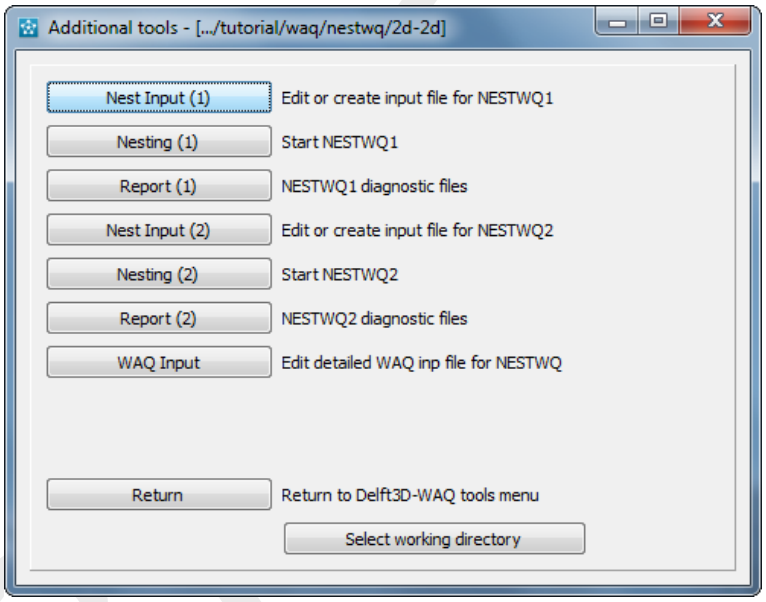


Figure 3.8: *Selection window for* ***Additional tools****, nesting water quality models*

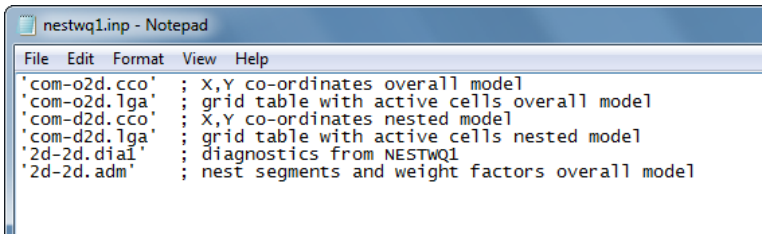


Figure 3.9: *Input file for NESTWQ1*

4 Input and output

NESTWQ1 and NESTWQ2 have each their own input file. The input files <nestwq1.inp> and <nestwq2.inp>, respectively, are free-formatted ASCII files.

4.1 Input NESTWQ1

The input file <nestwq1.inp> contains the following information:

<com-ext1.cco>	CHARACTER, the overall grid in X,Y co-ordinates at the depth locations
<com-ext1.lga>	CHARACTER, the table with (in)active segment numbers of the overall model
<com-ext2.cco>	CHARACTER, the nested grid in X,Y co-ordinates at the depth locations
<com-ext2.lga>	CHARACTER, the table with (in)active segment numbers of the nested model
<nestwq1.dia>	CHARACTER, diagnostics from NESTWQ1 and the required nest segments in D-Water Quality monitor format
<nestwq1.adm>	CHARACTER, per boundary segment the overall nest segments and weight factors required for the nesting procedure in NESTWQ2

The filenames between quotes are free to choose with a maximal length of 128 characters.

Remarks:

- ◇ The required information about the vertical structure of the models is contained in the grid files. If the overall model is 2DH and the nested model is 3D, NESTWQ2 will generate a uniform 3D profile for the nested model. If the overall model is 3D and the nested model is 2DH, NESTWQ2 will generate depth-averaged boundary conditions for the nested model.
- ◇ If both models are 3D then the number of layers in each model must be equal.

Example input file <nestwq1.inp>:

```
'..\hkcrs.3d\com-o3d.cco'   ; X,Y co-ordinates overall model
'..\hkcrs.3d\com-o3d.lga'   ; grid table with active cells overall model
'..\siulam.3d\com-d3d.cco'  ; X,Y co-ordinates nested model
'..\siulam.3d\com-d3d.lga'  ; grid table with active cells nested model
'3d-3d.dia'                 ; diagnostics from NESTWQ1
'3d-3d.adm'                 ; nest segments and weight factors overall model
```

4.2 Output NESTWQ1

The output files of NESTWQ1 are:

<nestwq1.dia>	the diagnostics from NESTWQ1 and the required nest segments in D-Water Quality monitor format
<nestwq1.adm>	per boundary segment the overall nest segments and weight factors required for the nesting procedure in NESTWQ2

Remarks:

- ◇ It is not necessary to include the required nest segments in the simulation with the overall model as the nesting is performed with the results in the map file. The map file contains the concentrations at every grid point, thus including the required nest segments.

◇ The administration file contains the required information about the vertical structure of each model.

See Chapter 5 for an example of these files.

4.3 Input NESTWQ2

The input file <nestwq2.inp> contains the following information:

<nestwq1.adm>	CHARACTER, the nest administration file with per boundary segment the overall nest segments and weight factors required for the nesting procedure in NESTWQ2
<d3d-waq.map>	CHARACTER, the map file with results from the overall model
nosys	INTEGER, the number of active substances to be nested
<nestwq2.dia>	CHARACTER, diagnostics from NESTWQ2
<ext.bcc>	CHARACTER, the boundary conditions at the (aggregated) boundary segments of the nested model

The filenames between quotes are free to choose with a maximal length of 128 characters.

Remark:

◇ The first 'nosys' active substances will be transferred as boundary conditions for the nested model.

Example input file <nestwq2.inp>:

```
'..\nestwq1.v20\3d-3d.adm'  ; nest segments and weight factors overall model
'o3d-waq.map'               ; map file overall model
   4                        ; number of active substances to nest
'3d-3d.dia'                 ; diagnostics from NESTWQ2
'3d3dwaq.bcc'               ; boundary conditions for nested model
```

4.4 Output NESTWQ2

The output files of NESTWQ2 are:

<nestwq2.dia>	the diagnostics from NESTWQ2
<ext.bcc>	the boundary conditions at the (aggregated) boundary segments of the nested model

See Chapter 5 for an example of the diagnostics file.

5 Tutorial

At this moment no graphical user interface is available to perform the nesting of water quality models. In order to perform the nesting, correctly, the following steps are required:

Edit/Create <nestwq1.inp> file for NESTWQ1
You have to specify the names of the <∗.lga> and <∗.cco> files of the overall and detailed model. Specify the administration file. On forehand the hydrodynamics of both the overall and nested model must be converted to formats required for D-Water Quality (Couple menu, see Deltares (2024a)).

Create administration file (execute NESTWQ1)
Within this step a diagnostic file and an administration file is created which is required input for the second step of the of the nesting (NESTWQ2).

Edit/Create <nestwq2.inp> file for NESTWQ2
You must specify the name of the administration file (created by step 2), the name of the water quality map file of the overall model , the number of active substances to nest and the name of the binary boundary output file for the detailed model.

Create boundary conditions (execute NESTWQ2)
Within this step a diagnostic file and a boundary file is created which is required input for running the water quality detailed model.

Examine diagnostic files of NESTWQ1 and NESTWQ2
After executing NESTWQ1 and/or NESTWQ2 you can inspect the if the modules have run correctly.

Edit nested WAQ input file
In this step you must add the created boundary filename (step 4) by editing block 4 of the water quality input file***:***

- ◇ goto block #4
- ◇ change *'1 : information in this file'* to *'-2 : information in binary file'*
- ◇ write on a new record the name of boundary file between quotes
- ◇ delete all other information in the following records in block #4 (until block #5)

In order to demonstrate the use of D-WAQ NESTWQ the following tutorial can be applied:

Available data files:

<com-d2d.dat>	: communication file detailed 2D model (Siu-Lam)
<com-d2d.def>	: definition file detailed 2D model
<com-o2d.dat>	: communication file overall 2D model (Upgrade 2x2)
<com-o2d.def>	: definition file overall 2D model
<tracer.sub>	: substance file with CTR1

1 Start Delft3D-MENU.
2 Select *Water Quality* from the main menu.
3 Select *General* from the **Far-field water quality (all modules)** selection window.
4 Select *Coupling* and start COUP-GUI by selecting *Define input*.
5 Open in COUP-GUI Data Group *Hydrodynamics* and open <com-02d.dat>.
6 Save the input as <com-o2d.hyd>.
7 Select *File – Exit* to leave COUP-GUI.

8 Select *Start* to execute the coupling. A window opens with messages from the coupling. Close this window when the coupling is finished.
9 Go back by selecting *Return* in the **Hydrodynamic coupling** window.
10 Select *Define input* to start the WAQ-GUI.
11 Activate in WAQ-GUI Data Group *Hydrodynamics* and select <com-02d.hyd> file.
12 Set dispersion to 10 m^2/s in x and y direction.
13 Activate Data Group *Substances* and select file <tracer.sub>.
14 Set Time Frame to 1-1-2000 - 3-1-2000 , timestep 3 minutes
15 Select Numerical option 5 in Data Group *Numerical options*
16 Add two discharges at (32,28) and (44,28) and assign a load of 1000 g/s of CTR1 to both discharges (Data Group *Discharges*) by button *Edit data*
17 Select *Output Option* Data Group and set output timers for the map file to 1-1-2000 (start) ; 3-1-2000 (stop) ; 1 hour time step
18 Save scenario as <∗.scn> file (e.g. <testo.scn>)
19 Exit the WAQ-GUI
20 Select *Waq (1)*; in selection window select scenario file, e.g. <testo.scn>.
21 Check report files on errors.
22 Select *Waq (2)* to start the calculation.
23 Visualise the results with Delft3D-QUICKPLOT or GPP (QUICKPLOT UM, 2018; GPP UM, 2013).
Repeat the above steps for the detailed model (<com-d2d.dat>) without step 16 and save the results in e.g. <testd.scn> (no discharges added).
24 Select *Tools* in the *Water quality (WAQ)* menu. The following menu will appear:

24.1 ***Edit or create input file for NESTWQ1***
You have to specify the names of the <∗.lga> and <∗.cco> files of the overall and detailed model conform the documentation (e.g. <com-o2d>, <com-d2d>). Specify administration file (e.g. <2d-2d.adm>).
24.2 ***Start NESTWQ1***
Within this step a diagnostic file and an administration file is created which is required input for the second step of the of the nesting (NESTWQ2)
24.3 ***Edit or create input file for NESTWQ2*** You must specify the name of the administration file (created by step 2), the name of the water quality map file of the overall model (e.g. <testo.map>), the number of active substances to nest and the name of the binary boundary output file for the detailed model (e.g. <2d-2d.bcc>).
24.4 ***Start NESTWQ2***
Within this step a diagnostic file and an boundary file is created which is required input for running the water quality detailed model.
24.5 ***Examine diagnostic files of NESTWQ1 and NESTWQ2***
24.6 ***Edit nested WAQ input file***
In this step you must add the created boundary file name (step 4) by editing block 4 of the water quality input file (e.g. <testd.inp>)

- ◇ goto block #4
- ◇ replace the block of lines starting with "ITEM" (right after the Thatcher-Harleman timelags for each boundary segment) up to (but not including) the line *#5 ; delimiter for the fifth block* by the *single* line *'-2 : information in binary file'*.
- ◇ write on a new record the boundary filename between quotes e.g. '2d-2d.bcc'
- ◇ delete all other information in the following records in block #4 (until block #5)

Note: You can also use the D-Water Quality user-interface: select the *Boundary Conditions* datagroup and press the *Data file* button. The dialogue that appears allows you to select the output file from NESTWQ2. This will then be included automatically in the input to D-Water Quality.
The advantage of this method is that the name of this output file becomes part of the

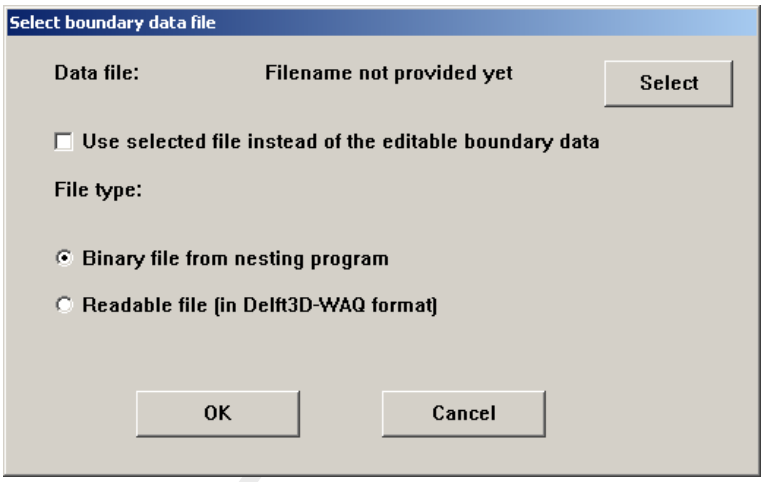


Figure 5.1: *Dialog for selecting output from NESTWQ2 in D-Water Quality GUI*

scenario and it will be included when you edit the input via the user-interface.

25 Return to **Water quality (WAQ)** menu and select *Waq (1)* and select the adapted <testd.inp> file.

26 Run the detailed model and evaluate the results.

5.1 Introduction

The Upgraded WAHMO Model is a fine-grid numerical model for the placeHong Kong waters. It is based on the shallow water equations in curvilinear co-ordinates. The spatial resolution is typical 300–1500 m. The model was developed in view of the need for a detailed and accurate tidal and water quality model that could be used for accurate computations. A further interest was provided by transport and water quality simulations on seasonal and annual scales. For this purpose the fine-grid water quality model was aggregated.

The SIU LAM model is a fine-grid numerical model for the waters north of Lantau Island. It uses a curvilinear fine grid. The hydrodynamic model was developed to investigate the effects of various layouts for a proposed typhoon shelter at Siu Lam.

As an example to demonstrate the nesting of water quality models a water quality model based upon the hydrodynamic SIU LAM model was set up.

For the generation of water quality boundary conditions for the WQ SIU LAM model, the model is nested in a coarse version of the WQ UPGRADE WAHMO model.

Figure 5.1 shows the coarse grid UPGRADE WAHMO together with the fine grid SIU LAM. The locations of the boundary segments of the SIU LAM model are presented in Figure 5.2.

In the following application grid cells have not been aggregated in both models. Both 3D models have 5 layers.

5.2 Input and output NESTWQ1

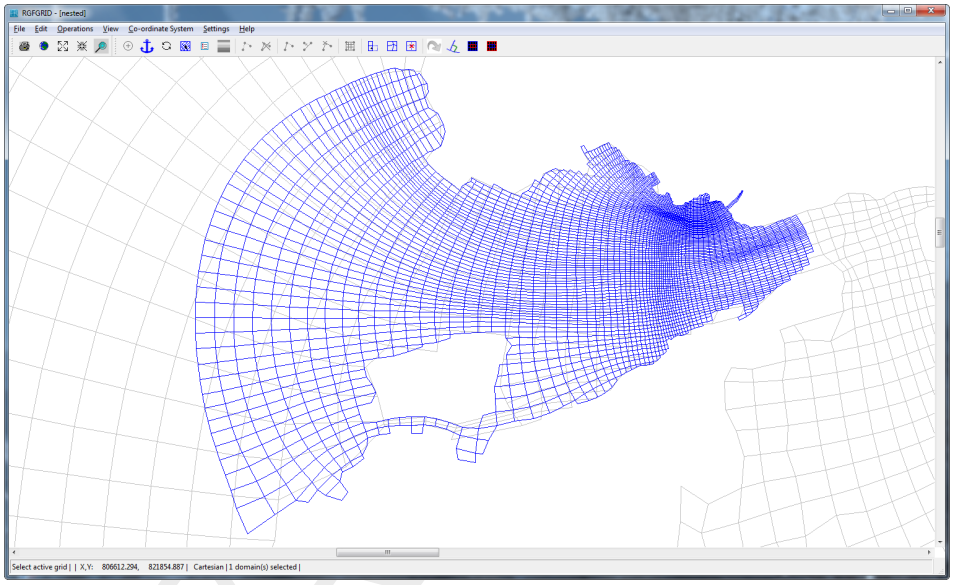


Figure 5.2: *Upgrade and Siu Lam models*

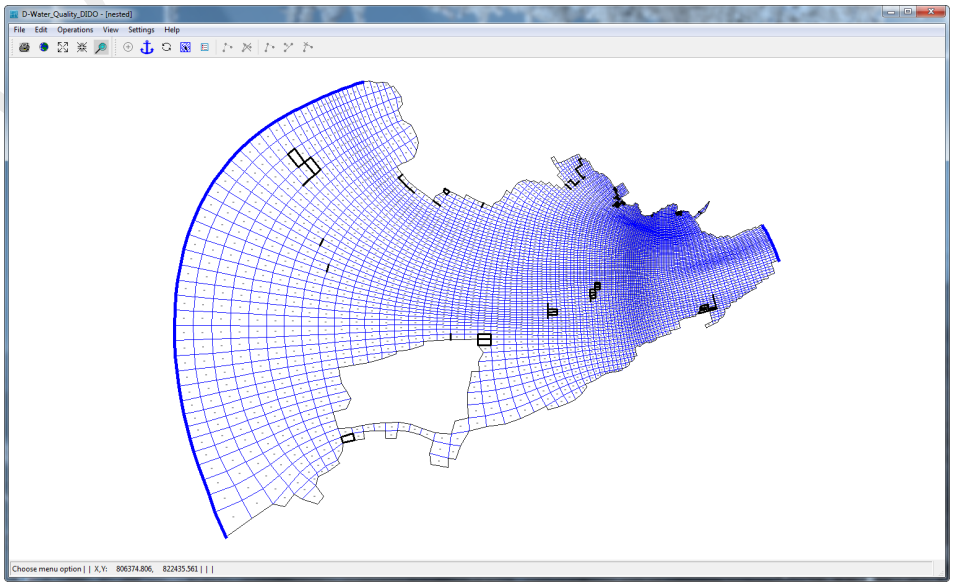


Figure 5.3: *Siu Lam model with 2 open boundaries (east and west)*

5.2.1 Input file

Input file <nestwq1.inp>:

```
'com-o2d.cco'  ; X,Y co-ordinates overall model
'com-o2d.lga'  ; grid table with active cells overall model
'com-d2d.cco'  ; X,Y co-ordinates nested model
'com-d2d.lga'  ; grid table with active cells nested model
'2d-2d.dia1'   ; diagnostics from NESTWQ1
'2d-2d.adm'    ; nest segments and weight factors overall model
```

5.2.2 Diagnostics file

Diagnostics file <2d-2d.dia1>:

```
Deltares, NESTWQ1 Version 2.04.02.25853, Jan 18 2013, 09:42:45

>> Input from nestwq1.inp

X,Y co-ordinates overall model               : com-o2d.cco
Grid table with active cells overall model   : com-o2d.lga
X,Y co-ordinates nested model                : com-d2d.cco
Grid table with active cells nested model    : com-d2d.lga

Diagnostics and required nest segments       : 2d-2d.dia1
Nest segments and weight factors overall model : 2d-2d.adm

Weight factors for boundary   -1 aggr. no.=     1
  1:          0.4713E+00
  2:          0.2868E+00
  3:          0.9152E-01
  4:          0.1504E+00

Weight factors for boundary   -2 aggr. no.=     1
  1:          0.6820E+00
  2:          0.9224E-01
  3:          0.2690E-01
  4:          0.1989E+00


...


*** WARNING *** negative 3rd weight for    -9    1

*** WARNING *** negative 4th weight for    -9    1

...

Weight factors for boundary  -68 aggr. no.=     1
  1:          0.4379E+00
  2:          0.2572E+00
  3:          0.1128E+00
  4:          0.1921E+00

>> List of required nest segments in Delft3D-WAQ monitor format

Number of required nest segments             :   51

 1719 'Nest segment   1719 ' 1720 'Nest segment   1720 ' 1782 'Nest segment   1782 '
 1781 'Nest segment   1781 ' 1780 'Nest segment   1780 ' 1718 'Nest segment   1718 '
 2897 'Nest segment   2897 ' 2959 'Nest segment   2959 ' 1779 'Nest segment   1779 '
 1717 'Nest segment   1717 ' 2958 'Nest segment   2958 ' 2896 'Nest segment   2896 '
 1778 'Nest segment   1778 ' 1716 'Nest segment   1716 ' 2957 'Nest segment   2957 '
```

```
 2895 'Nest segment   2895 ' 1654 'Nest segment   1654 ' 1655 'Nest segment   1655 '
 1715 'Nest segment   1715 ' 1653 'Nest segment   1653 ' 1714 'Nest segment   1714 '
 1652 'Nest segment   1652 ' 1713 'Nest segment   1713 ' 1651 'Nest segment   1651 '
 2956 'Nest segment   2956 ' 2894 'Nest segment   2894 ' 1712 'Nest segment   1712 '
 1650 'Nest segment   1650 ' 1711 'Nest segment   1711 ' 1649 'Nest segment   1649 '
 1710 'Nest segment   1710 ' 1648 'Nest segment   1648 ' 1709 'Nest segment   1709 '
 1647 'Nest segment   1647 ' 1771 'Nest segment   1771 ' 1770 'Nest segment   1770 '
 1708 'Nest segment   1708 ' 1769 'Nest segment   1769 ' 1707 'Nest segment   1707 '
 1768 'Nest segment   1768 ' 1706 'Nest segment   1706 ' 1830 'Nest segment   1830 '
 1829 'Nest segment   1829 ' 1767 'Nest segment   1767 ' 1828 'Nest segment   1828 '
 1766 'Nest segment   1766 ' 1890 'Nest segment   1890 ' 1889 'Nest segment   1889 '
 1827 'Nest segment   1827 ' 1888 'Nest segment   1888 ' 1826 'Nest segment   1826 '

>> Number of warnings          :     6

>> Number of error messages    :     0
```

5.2.3 Administration file

Nest administration data file <2d-2d.adm> (only a part is given):

```
Deltares, NESTWQ1 Version 2.04.02.25853, Jan 18 2013, 09:42:45

>> Files used to determine nest characteristics

X,Y co-ordinates overall model                : com-o2d.cco
Grid table with active cells overall model    : com-o2d.lga
Number of segments overall model per layer    :   4774
Number of layers overall model                :      1
X,Y co-ordinates nested model                 : com-d2d.cco
Grid table with active cells nested model     : com-d2d.lga
Number of segments nested model per layer     :   7400
Number of layers nested model                 :      1

>> List of boundary segments, required nest segments and weight factors

Nest model  Overall model
----------  --------------
SEGNR #NST  SEGNR   WEIGHT
   -1    4   1719  0.47127
             1720  0.28682
             1782  0.09152
             1781  0.15038
SEGNR #NST  SEGNR   WEIGHT
   -2    4   1719  0.68195
             1720  0.09224
             1782  0.02690
             1781  0.19890

...

SEGNR #NST  SEGNR   WEIGHT
  -68    4   1827  0.43793
             1889  0.25716
             1888  0.11281
             1826  0.19211
```

5.3 Input and output NESTWQ2

5.3.1 Input file

Input file <nestwq2.inp>:

```
'2d-2d.adm'     ; nest segments and weight factors overall model
'o2d-waq.map'   ; WAQ map file overall model
   4            ; number of active substances for nested model
'2d-2d.dia2'    ; diagnostics from NESTWQ2
'2d2dwaq.bcc'   ; WAQ boundary conditions for nested model
```

5.3.2 Diagnostic file

The diagnostics file <2d-2d.dia2>:

```
Deltares, NESTWQ2 Version 2.04.00.25853, Jan 18 2013, 09:42:44

>> Input from nestwq2.inp

Nest segments and weight factors overall model : 2d-2d.adm
Map file overall model                         : o2d-waq.map
Number of active substances to nest            :   4

Diagnostics NESTWQ2                            : 2d-2d.dia2
Boundary conditions for nested model           : 2d2dwaq.bcc

Deltares, NESTWQ1 Version 2.04.02.25853, Jan 18 2013, 09:42:45

>> Files used to determine nest characteristics

X,Y co-ordinates overall model                 : com-o2d.cco
Grid table with active cells overall model     : com-o2d.lga
Number of segments overall model per layer     :   4774
Number of layers overall model                 :      1
X,Y co-ordinates nested model                  : com-d2d.cco
Grid table with active cells nested model      : com-d2d.lga
Number of segments nested model per layer      :   7400
Number of layers nested model                  :      1

>> Delft3D-WAQ map file characteristics

Model and run identification   : 1- Delft3D-WAQ ---------------------- 1
                                 2- Upgrade WAHMO coarse model -------- 2
                                 3- test ------------------------------ 3
                                 4- map results to nest SIU LAM ------- 4

Total number of variables      :      7

Variable names on map file     : Substance  1
                                 Substance  2
                                 Substance  3
                                 Substance  4
                                 Inactive subst  5
                                 Inactive subst  6
                                 Extra variable  7

Selected variables to nest     : Substance  1
                                 Substance  2
                                 Substance  3
                                 Substance  4

Total number of segments       :   4774

>> Number of warnings          :     0
```

```
>> Number of error messages     :      0
```

6 Limitations, warnings and errors

6.1 Limitations

- The X,Y co-ordinates of the overall grid and the nested grid are stored in so-called (binary) cco-files. These files are platform dependent.
- The overall and nested grid have the same co-ordinate system.
- The time-series boundary conditions for the (aggregated) nested model are derived from the binary D-Water Quality map file from the (aggregated) overall model.
- The first NOSYS active substances on the map file of the overall model are transferred to the nested model; selection of substances is not possible.
- The location of a boundary segment in the nested model is obtained through mirroring from the interior domain.
- The centre of a boundary segment in the nested model before aggregation, and the centres of the surrounding overall nest segments determine the weight factors.
- The nest procedure transfers 2DH and 3D overall model results to 2DH and 3D boundary conditions for the nested model. In case both models are 3D then the number of layers in both models must be equal. 2DH overall model results will be transformed to uniform 3D boundary conditions for the nested model. 3D overall model results will be transformed to depth-averaged boundary conditions if the nested model is 2DH.
- The time-series boundary conditions file for the nested model is binary and only suitable for D-Water Quality.
- The time span and time interval for the time-series boundary conditions of the nested model are determined by the map time span and interval of the map file from the overall model.
- The nesting procedure D-WAQ NESTWQ does not account for drying in the overall model.
- If there are missing boundary segment numbers (gaps in the numbering) they will get the value 0.0 as concentration in the boundary conditions file.

6.2 Warnings

Warnings from subsystem NESTWQ1 can be:

```
*** WARNING *** centre of boundary segment -xxxxx, (M,N) = (xxx,xxx)
                            not inside a nest segment
                            the nearest nest segment will be taken
```

When the centre of a boundary segment is not inside the polygon spanned by the centres of the nest segments, extrapolation takes place. This may cause one or more negative weight factors. Consequently, this may lead to negative concentrations. To avoid this, NESTWQ2 will reset negative concentrations to 0.0. The following four warnings may occur:

```
*** WARNING *** negative 1st weight for -xxx xxx

*** WARNING *** negative 2nd weight for -xxx xxx

*** WARNING *** negative 3rd weight for -xxx xxx

*** WARNING *** negative 4th weight for -xxx xxx
```

When the sequence of boundary segment numbers is interrupted, the following warning is issued. In the time-series file for the nested model a missing boundary segment will have zero concentrations.

```
*** WARNING *** boundary segment -xxx is missing
```

NESTWQ2 gives no warnings.

6.3 Errors

Errors from subsystem NESTWQ1 can be:

```
*** ERROR *** The file nestwq1.inp does not exist
```

The following error is related to missing grid or segment numbers files.

```
*** ERROR *** non-existing file
```

If the format or structure of the input, <*.cco> or <lgrid> files is incorrect, the following errors will be given.

```
*** ERROR *** while reading nestwq1.inp

*** ERROR *** premature EOF nestwq1.inp

*** ERROR *** while reading <com-ext.cco>

*** ERROR *** premature EOF <com-ext.cco>

*** ERROR *** while reading <com-ext.lga>

*** ERROR *** premature EOF <com-ext.lga>
```

The following dimensions may be too small; they can be increased in the main program.

```
*** ERROR *** increase MNMAX to xxxxx

*** ERROR *** increase MAXBND to xxxxx

*** ERROR *** increase MAXAGR to xxxxx

*** ERROR *** increase MAXNST to xxxxx
```

When the <*.cco> or <*.lga> file mismatch, the errors are:

```
*** ERROR *** inconsistent MMAX
                         MMAX-cco = xxxxx
                         MMAX-lga  = xxxxx

*** ERROR *** inconsistent NMAX
                         NMAX-cco = xxxxx
                         NMAX-lga  = xxxxx

*** ERROR *** inconsistent LAYT
                          LAYT-cco = xxxxx
                          LAYT-lga  = xxxxx
```

The next two errors may not occur (when they occur your data files were corrupted).

```
*** ERROR *** increase NMAX in pinpol to xxxx

*** ERROR *** number of nest segments : xxxxx
                        at boundary segment -xxx xxx
```

Failures in the determination of the weight factors may cause the errors:

```
*** ERROR *** singular points for ichoic = x

*** ERROR *** no convergence newton-raphson iteration ichoic = xxx
```

Errors from subsystem NESTWQ2 can be:

```
*** ERROR *** The file nestwq2.inp does not exist
```

The following error is related to missing nest administration data from NESTWQ1 or D-Water Quality map file.

```
*** ERROR *** non-existing file
```

If the format or structure of the input, nest administration or D-Water Quality map file is incorrect, the following errors will be given.

```
*** ERROR *** while reading nestwq2.inp

*** ERROR *** premature EOF nestwq2.inp

*** ERROR *** while reading <nestwq1.adm>

*** ERROR *** premature EOF <nestwq1.adm>

*** ERROR *** while reading <d3d-waq.map>

*** ERROR *** premature EOF <d3d-waq.map>
```

The following dimensions may be too small; they can be increased in he main program.

```
*** ERROR *** increase MAXVAR to xxxxx

*** ERROR *** increase MAXSYS to xxxxx

*** ERROR *** increase MAXBND to xxxxx

*** ERROR *** increase MAXAGR to xxxxx

*** ERROR *** increase MAXSEG to xxxxx
```

When there is an inconsistency between the files used for NESTWQ1 and the overall map file used in NESTWQ2 the error will be:

```
*** ERROR *** inconsistent number of segments
                         NOSEG from NESTWQ1 = xxxxx
                         NOSEG from mapfile        = xxxxx
```

An inconsistency in the number of layers for 3D models will cause the error:

```
*** ERROR *** 3D-3D nesting with different number of
                         layers is NOT implemented
```

7 Description files

The files used by NESTWQ1 and NESTWQ2 are described as follows.

Name: <com-ext1.cco>, <com-ext2.cco>
Type: binary
Access: transparent
Contents:
1 empty record
2 2 integers; 3 reals, 2 integers; MMAX, NMAX, XCOR1, YCOR1, 0.0, 0, LAYT
1 9 records with 0.0
12 NMAX*MMAX reals; (X(k), k=1,NMAX*MMAX)
13 NMAX*MMAX reals; (Y(k), k=1,NMAX*MMAX)

Name: <com-ext1.lga>, <com-ext2.lga>
Type: binary
Access: transparent
Contents:
1 7 integers; NMAX, MMAX,NMNW,LAYT, NOQ1, NOQ2, NOQ3
2 NMAX*MMAX integers; (LGRID(k), k=1,NMAX*MMAX)

Name: <nestwq1.dia>
Type: ASCII
Format: free-formatted
Contents: the file contains information about:

- subsystem name and version number
- the names of the input and output files of NESTWQ1
- the required (overall) segments in D-Water Quality monitor format
- warnings and errors occuured while executing NESTWQ1

Name: <nestwq1.adm>
Type: ASCII
Format: free-formatted
Contents: the file contains information about:

- subsystem name and version number
- the filenames which have been used in the nesting procedure
- the number of segments per layer in both models
- the number of layers in both models
- per boundary segment the required (overall) nest segments and their weight factors

Name: <d3d-waq.map>
Type: binary
Access: transparent
Contents:
1 4 * character * 40 model and run id
2 2 integers NOVAR and NOSEG
3 NOVAR * character * 20 variable names
4 for each time step, an integer and NOVAR * NOSEG reals;
itime ((CONC(ivar,iseg),ivar=1,NOVAR),iseg=1,NOSEG)

Name: <nestwq2.dia>
Type: ASCII
Format: free-formatted
Contents: the file contains information about:

- subsystem name and version number

- the names of input and output files used by NESTWQ2
- the number of active substances
- the names of input files used by NESTWQ1
- model and run identification of the simulation with the overall model
- total number of variables on the map file
- variable names on the map file
- selected variables to nest
- warnings and errors occurred while executing NESTWQ2

Name: <ext.bcc>
Type: binary
Access: transparent
Contents: for each time step, an integer and NOSYS * NOBND reals;

itime ((CONC(isys,ibnd),isys=1,NOSYS),ibnd=1,NOBND)

8 Theoretical background

8.1 Boundary segments

Boundary segments are segments with a negative segment number. In case of an aggregated grid, there may be more than one boundary segment with the same negative number. Normally, when aggregation is done, interior grid cells will be aggregated; the boundary segments will not be aggregated.

In the nesting procedure the time-series from the nest segments are interpolated to the centre of each (individual) boundary segment. If boundary segments are aggregated these interpolated time-series are then averaged over the boundary segments with the same segment number.

8.2 Nest segments and weights

The centre of each boundary segment determines in which (overall) nest segment the centre is located. Depending on the quadrant within this nest segment, maximal three other adjacent nest segments are determined. It may be possible that 3, 2, 1 or no other nest segments can be specified. For instance, when the first nest segment is at the edge of the overall grid, only 1 additional nest segment may be identified.

When the centre of a boundary segment is not included in any overall segment then the nearest overall segment is taken as the only nest segment. The criterion for the nearest segment is that segment with the shortest distance between its centre and the centre of the boundary segment.

The centres of the nest segments and the centre of the boundary segment determine the weights for each nest segment. The options are linear (2 and 3 nest segments) and bi-linear (4 nest segments) interpolation.

References

Deltares, 2024a. *D-Water Quality User Manual*. Deltares, 5.06 ed.

Deltares, 2024b. *Delft3D-PART User Manual*. Deltares, 2.13 ed.

GPP UM, 2013. *Delft3D-GPP User Manual*. Deltares, 2.14 ed.

QUICKPLOT UM, 2018. *Delft3D-QUICKPLOT User Manual*. Deltares, 2.30 ed.

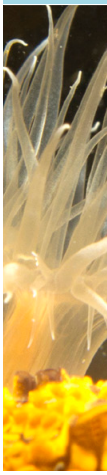


Photo by: Mathilde Matthijsse, www.zeelandonderwater.nl

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