

Simulation software for safe, sustainable and future deltas

# DELFT3D FM SUITE 2D3D

Deltares systems

D-Water Quality Tools



# **D-Water Quality tools**

**Purpose and use of the programs**

**User Manual**

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## D-Water Quality tools, User Manual

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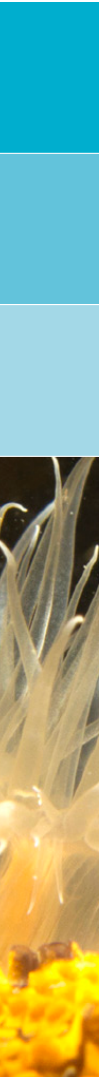
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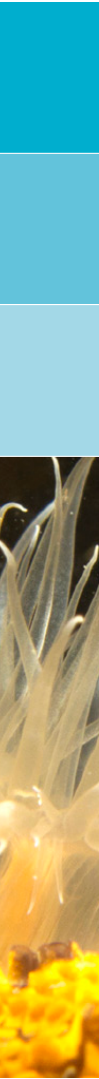


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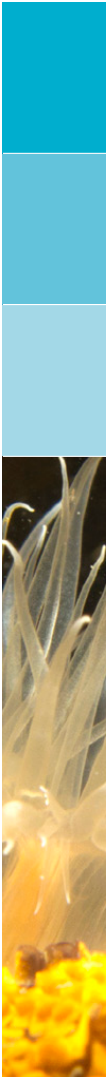


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# 1 Agrhyd

## 1.1 Introduction

The requirements with regards to the horizontal and vertical resolution of the computational grid for water quality calculations do not always coincide with the requirements for hydrodynamic modelling. Quite often it is necessary for a hydrodynamic model to have a high horizontal and vertical resolution, whereas the gradients in the water quality parameters are much "lazier". Using a large number of vertical layers then becomes a computational burden. The same is true for very detailed grids needed to resolve the bottom topography.

The net result is that it is often beneficial to aggregate the grid and the hydrodynamic results that based on the grid before running a water quality model. This is the purpose of the Agrhyd program. Horizontal aggregation is in general prepared via the D-WAQ DIDO program, as this allows you define the aggregation using a graphical user-interface. Vertical aggregation is prepared using a simple text file.

Currently, Agrhyd is capable of processing Delft3D-FLOW and D-Flow FM hydrodynamic data sets. Data sets that produce the hydrodynamic data set in the same formats might also be processed, however, this has not yet been tested.

In addition the Agrhyd program is capable of concatenating various hydrodynamic databases that are based on the same grid from Delft3D-FLOW runs that were restarted (keyword `inputhydpatch`, `inputhydpatch1`, `inputhydpatch2`, etc).

## 1.2 Input parameters

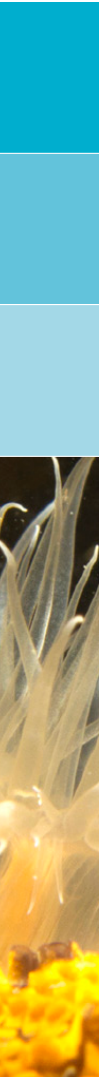
The program takes as an argument the name of the input file (formatted as a so-called INI-file). The keywords need to appear below the "chapter" "[General]".

Here is an example:

```
[General]
inputhyd           = com-test.hyd
output             = com-test2
vertical_aggregation_file = from_25_to_10layers.inp
```

Notes:

- ◇ The program supports both structured curvilinear grids (such as provided by Delft3D-FLOW) and unstructured grids (as from D-Flow FM), but regular aggregation and expansion are only possible for structured grids.
- ◇ If you specify a file for horizontal aggregation, then you cannot also specify regular aggregation.
- ◇ Concatenation of hydrodynamic databases requires that they are based on the same hydrodynamic grid and if aggregation has been applied within the hydrodynamic calculation, then the aggregation specification must be the same for all.  
This is checked only rudimentary, so you may have to be careful.



**Table 1.1:** Keywords in the input file for agrhyd.

<i>Keyword</i>	<i>Purpose</i>	<i>Default</i>
<i>File names</i>		
inputhyd	Name of the hyd-file (input)	required
inputhydpatch	Name of an additional hyd-file (input)	optional
inputhydpatch1	Name of a second additional hyd-file (input)	optional
inputhydpatch2	Ditto, these hydrodynamic results are appended	optional
...	to the very first result (see text below)	optional
inputhydpatch9	Name of a ninth additional hyd-file (input)	optional
horizontal_aggregation_file	Name of an aggregation file (.dwq)	optional
vertical_aggregation_file	Name of a file to aggregate layers	optional
output	Name for the output files	required
<i>Regular aggregation</i>		
expand	Expand the grid (disaggregate)	false
regular	Whether regular aggregation is defined here (for structured curvilinear grids only)	false
m_fact	Number of cells taken together in first (m) direction	–
n_fact	Number of cells taken together in second (n) direction	–
m_offset	Offset for starting aggregation in first (m) direction	–
n_offset	Offset for starting aggregation in second (n) direction	–
<i>Other parameters</i>		
lenlen	Do not recalculate the dispersion length	false
minimum-dispersion-length	Minimum length for dispersion	0.0 m
start	Start time for output (default to start of files)	–
stop	Stop time for output (default to end of files)	–
reference_time_output	New reference time (calendar date/time)	–

The vertical aggregation, i.e. taking layers together is specified via a simple file, containing on the first line the number of layers in the hydrodynamic model and on subsequent lines the indices of the water quality layer for each hydrodynamic layer. For instance:

```
10           (Number of layers in the hydrodynamic model)
1 1 1 2 2 2 3 3 3 3
```

This example states that the first three layers in the hydrodynamic model should be put into the first water quality layer, then the next three in the second water quality layer, and the final four in the third water quality layer. You are yourself responsible for making sure that the layer numbering is consistent.

### 1.3 Output files

The program will write a number of output files:

- ◇ A new hyd-file, which contains the names of the new files, resulting from the aggregation and concatenation of the original hydrodynamic files.
- ◇ A report file with suffix "-agrhyd.rep"

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## 2 DD Couple

### 2.1 Introduction

When using a domain decomposed into several domains, the data needs to be coupled for further usage. The tool DD Couple couples the data from several domains into one domain. It can handle both classic DD output as MPI-based parallel Delft3D FLOW output.

### 2.2 Input

The program takes as an argument a "<input>.ddb" file. For MPI-based parallel Delft3D FLOW output, you must add the -parallel (or the shorthand -p) to let DD Couple properly reconstruct the grid as if the model had run as a single domain.

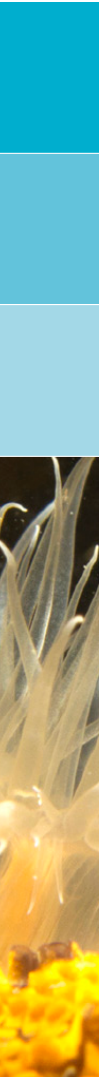
The input files are given by "com-<input>-xxx.<ext>" where typical extensions include ".are", ".flo", ".sal", ".tau", ".tem", ".vdf", ".vol", ".len", ".atr", ".poi", ".src", ".dps", ".srf", ".cco", ".lga" and ".hyd" files. The "xxx" indicates the domain number.

The program can be run using the "run\_ddcouple.bat" or "run\_ddcouple.sh" scripts provided in the installation.

### 2.3 Output files

The program will write a number of output files:

- ◇ A new set of files: "com-<input>.<ext>", with again the typical extensions such as: ".are", ".flo", ".sal", ".tau", ".tem", ".vdf", ".vol", ".len", ".atr", ".poi", ".src", ".dps", ".srf", ".cco", ".lga" and ".hyd".
- ◇ A report file "<input>-ddcouple.log".



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## 3 Waqmerge

### 3.1 Introduction

When using multiple partitions, D-Flow FM will create an output folder with several sets of files, one per partition.<sup>1</sup> Since D-Water Quality can accept results for a single partition only, the results have to be merged into one. The tool Waqmerge performs this merge.

### 3.2 Input

The program takes as an argument the modelname of the simulation. The results from D-Flow FM are written into an specific output folder with the default name "DFM\_DELWAQ-<modelname>". The name can be modified by setting the keyword "WAQOutputDir" in the "output" section of "<modelname>.mdu".

It examines the contents of the folder holding the output files from D-Flow FM, that is, it counts the files with names like "<modelname>0000.hyd", "<modelname>0001.hyd", etc. that are present. This number is taken as the number of partitions (see also Section 3.4).

### 3.3 Output files

The program will write several output files:

- ◇ In the folder "DFM\_DELWAQ-<modelname>" or the one identified by the keyword "WAQOutputDir" in the "<modelname>.mdu", containing the merged output of D-Flow FM. This merged output does not have a partition number:
  - D-Flow FM writes the files specific to a partition with a name like "runid\_0000.vol", "runid\_0001.vol", ...
  - Waqmerge writes the files for the merged model with a name like "runid.vol", that is the partition number is dropped.
- Use the "hyd" file "runid.hyd" to work with the overall model.
- ◇ A report file with suffix "-waqmerge.log".

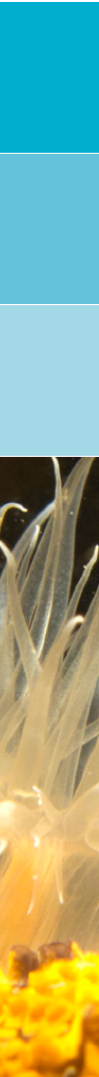
### 3.4 Caveats and limitations

For a proper use of the current version of the Waqmerge program several things must be kept in mind:

- ◇ The merged hydrodynamic database is *not* suitable for the D-Particle Tracking program (yet). This is due to the organisation of the file that holds the grid information, the so-called "waqgeom" file. Only hydrodynamic databases from a single-partition calculation should be used with D-Particle Tracking.<sup>2</sup>
- ◇ If a calculation for the same model input is redone but with a smaller number of partitions, the output directory may contain result files left over from the previous calculation. The Waqmerge program has no way of knowing this and will try and combine all hydrodynamic files from both calculations. The proper way of dealing with this is to first remove the output directories before restarting the calculation. (This holds for the map files from D-Flow FM as well, so it is an issue that should be solved within D-Flow FM.)
- ◇ The boundary information, that is the numbering of the open boundaries in D-Water Quality as derived from the grid information that Waqmerge produces for the merged, overall,

<sup>1</sup>Older versions of D-Flow FM might produce multiple output folders, one for each partition, if you did not specify the folder to which the files should be written

<sup>2</sup>The reason for this limitation is that the administration of the edges and nodes has to be reconstructed for the grid as a whole from the administration per partition and this is a rather complicated procedure.



grid, depends on the number of partitions. As long as that number remains the same, the numbering is correct, but if a different number of partitions is used, then the numbering changes and it is necessary to revise existing input for D-Water Quality. Note that this is only required for the open boundaries. The segment numbers, used for the monitoring locations and the waste load locations, as well as for the spatially varying process parameters, are independent of the partitioning, as Waqmerge uses the internal global numbering from D-Flow FM. Such a numbering is not available for the open boundaries.

In less technical terms:

- ◇ Do not use multi-partition hydrodynamic calculations for D-Particle Tracking.
- ◇ Remove the D-Flow FM output directories whenever you restart a calculation.
- ◇ Take care of the boundary numbering in existing D-Water Quality input files, if the number of partitions changes.

## 4 Flocheck

### 4.1 Introduction

D-Water Quality offers a wide variety of integration methods and options to these methods. Roughly the methods fall into two categories: implicit and explicit methods. While the implicit methods are usually preferable over explicit methods, sometimes there are good reasons to choose an explicit method nonetheless.

The big advantage of implicit methods is that they are inherently stable, that is, you can take any time step you want. The disadvantage is that they may use more memory than is available on the machine (with big models and/or a lot of computational threads) and that the calculation may be slow because large systems of matrices have to be solved.

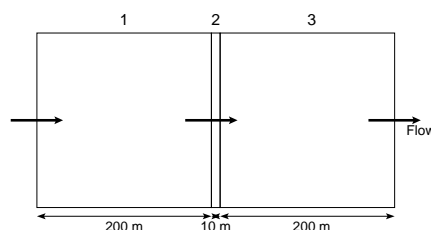
The advantage of explicit methods is that they tend to be fast and do not use much extra memory. The disadvantage is that there is a limit on the time step because of the stability criteria that have to be met. Normally, that is not a significant problem, but it may happen that a few small segments in the model schematisation hinder the application of explicit methods. Consider the simplified situation in [Figure 4.1](#).

The middle segment in the model schematisation is very small in comparison to the other two and therefore it determines the maximum allowable time step. Given the flow rates and volumes, the maximum time step imposed by the two large segments is 1000 s, but the small segment requires a time step of at most 50 s. This is merely an example, but this is a typical situation in 2D and 3D models, where segments in shallow areas may have a small surface area but still experience a large flow velocity.

One way to solve this is to join such segments with large neighbouring segments via the D-WAQ DIDO program. In a large model this can be very tedious work and then the Flocheck program may be useful, as this automatically adjusts the volumes so that a more reasonable time step can be used.

The program determines the volume adjustment based on a requested time step and a requested minimum volume for each segment. It then adjusts the volumes over time with this constant value. The criteria it uses are:

- ◇ The volume in a segment must be at least the given minimum. This is to avoid very shallow segments that might arise in areas with tidal flats.
- ◇ The volume in a segment must be large enough to support the requested time step. For this stability criterium, basically the Courant-Friedrichs-Lewy condition: "The volume of water replaced within any grid cell within one time step should always be smaller than the volume of the grid cell."



**Figure 4.1:** Sketch of a model schematisation with three segments. The middle segment is much smaller than the other two, giving rise to a much more severe restriction on the time step.

Based on the analysis of the hydrodynamic database with respect to these criteria the program writes a new volumes file that contains the adjusted volumes. With this alternative the explicit integration methods can be safely used.

## 4.2 Input parameters

The program takes as an argument the name of the input file (formatted as a so-called INI-file). The keywords need to appear below the "chapter" "[General]".

**Table 4.1:** Keywords in the input file for flocheck.

Keyword	Purpose	Default
inputhyd	Name of the hyd-file (input)	required
output	Name for the output files	required
idt	Requested time step (in seconds)	required
hdisp1	Horizontal dispersion (first direction)	1 m <sup>2</sup> /s
hdisp2	Horizontal dispersion (second direction)	1 m <sup>2</sup> /s
noflow_nodisp	Do not apply dispersion if flow rate is zero	true
vmin	Requested minimum volume	1.0 m <sup>3</sup>
dmin	Requested minimum depth	0.0 m
massbal_extra	Write extra information about the mass balance	false
vcheck	Limit on volume balance error for reporting	1.0 · 10 <sup>-7</sup> m <sup>3</sup>
qcheck	Limit on volume balance error as flow rate	1.0 · 10 <sup>-6</sup> m <sup>3</sup> /s
correct_flow	Correct the flow for balance errors	false
correct_flow_up	Use the vertical flow to correct balance errors	false
bagger_map	Name of a file with the "depth" corrections for all segments	not used
bagger2d_map	Name of a file with the "depth" corrections per water column (total over the column)	not used
missing_src	Name of a file to which the discharge rates are written as determined from the volume balance	not used

Here is an example:

```
[General]
inputhyd      = agr-com-test.hyd
output        = agr-com-test2
idt           = 300
hdisp1        = 1.0
hdisp2        = 1.0
noflow_nodisp = true
vmin          = 200.
```

It shows how to specify the logical values `true` and `false`.

### 4.3 Output files

The program will write a number of output files:

- ◇ A new hyd-file, which contains the name of the new files with adjusted volumes and possibly adjusted flows. This can be used as an alternative.
- ◇ A new volumes file with the adjustments to the volumes.
- ◇ A new flows file, if requested, with the adjustments to the flows.
- ◇ Two report files:
  - The file with suffix `-flocheck.rep` contains a report of the input and an overview of the adjustments that were made.
  - The file with suffix `-massbal.rep` contains a detailed report on mass balance errors for those segments where such errors were encountered.

### 4.4 Suggestions for use

In principle you do not want too much adjustments in the hydrodynamic database. Therefore it is important to use input parameters that minimize them:

- ◇ Choose time step that is not too large. The larger the time step, the more likely it is that the volume of a segment must be adjusted to meet the stability criterium.
- ◇ Similarly use a small enough value for the required minimum volume.
- ◇ Use the reports to check that not too much has been changed.

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