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Technical Reference Manual

Water Quality Modelling

Using the mass balances facilities

User Manual

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Version: 5.01
SVN Revision: 52847

November 23, 2017

Water Quality Modelling, User Manual

Published and printed by:
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1 Principles

1.1 Basic equations and definitions of mass balances

The central equation of DELWAQ is the advection diffusion equation, which we can express as follows for one state variable and for one segment:

$$\frac{dM}{dt} = T(t) + W(t) + P(t) \tag{1.1}$$

where

M	mass of state variable [g]
t	time [s]
T	change of mass as a result of transport [g/s]
W	change of mass as a result of waste loads [g/s]
P	change of mass as a result of processes [g/s]

If we integrate this equation over a certain period of time, say from $t = t_1$ to $t = t_2$, we can express the result as follows, again for one state variable and for one segment:

$$M(t_2) - M(t_1) = \int_{t_1}^{t_2} T(t)\ dt + \int_{t_1}^{t_2} W(t)\ dt + \int_{t_1}^{t_2} P(t)\ dt \tag{1.2}$$

or

$$M(t_2) - M(t_1) = T_{1\to 2} + W_{1\to 2} + P_{1\to 2} \tag{1.3}$$

or

$$0 = T_{1\to 2} + W_{1\to 2} + P_{1\to 2} + \underbrace{M(t_1) - M(t_2)}_{\text{storage}} \tag{1.4}$$

The mass balances feature of DELWAQ presents the results from the simulation, from $t = t_1$ to $t = t_2$, as follows:

```
============================================================
Mass balances for segment X
============================================================
Substance Y                    Sources/Inflows Sinks/Outflows
------------------------------------------------------------
Storage  (M(t1) - M(t2))                     0             0
Transport (T1-->2)                           0             0
Waste loads (W1-->2)                         0             0
Processes (P1-->2)                           0             0
SUM OF ALL TERMS                             0             0
```

Note:

1. The storage term represents the change of the mass during the simulation. We can also use the word “accumulation”. Following the basic equation, the storage term in the balance is expressed as $M(t_1) - M(t_2)$. This implies that the storage term is positive if the mass decreases with time and vice versa. In other words:
   storage $\equiv$ decrease of mass (!)
2. The positive and negative terms are provided in separate columns.
3. The sum of all numbers in both columns is provided, for easy checking.

1.2 Basic examples

Below a few basic examples are presented. The absolute values of the numbers do not have a meaning in this case.

Inflow of pollutants leading to an increase of mass:

```
============================================================
Mass balances for segment X
============================================================
Substance Y                    Sources/Inflows Sinks/Outflows
------------------------------------------------------------
Storage  (M(t1) - M(t2))                 0            -100
Transport (T1-->2)                     100               0
Waste loads (W1-->2)                     0               0
Processes (P1-->2)                       0               0
SUM OF ALL TERMS                       100            -100
```

Outflow of pollutants leading to a decrease of mass:

```
============================================================
Mass balances for segment X
============================================================
Substance Y                    Sources/Inflows Sinks/Outflows
------------------------------------------------------------
Storage  (M(t1) - M(t2))               100               0
Transport (T1-->2)                       0            -100
Waste loads (W1-->2)                     0               0
Processes (P1-->2)                       0               0
SUM OF ALL TERMS                       100            -100
```

Waste loads balanced by outflow of mass (steady state):

```
============================================================
Mass balances for segment X
============================================================
Substance Y                    Sources/Inflows Sinks/Outflows
------------------------------------------------------------
Storage  (M(t1) - M(t2))                 0               0
Transport (T1-->2)                       0            -100
Waste loads (W1-->2)                   100               0
Processes (P1-->2)                       0               0
SUM OF ALL TERMS                       100            -100
```

Decay of pollutant (no loads or transport):

```
============================================================
Mass balances for segment X
============================================================
Substance Y                    Sources/Inflows Sinks/Outflows
------------------------------------------------------------
Storage  (M(t1) - M(t2))               100               0
Transport (T1-->2)                       0               0
Waste loads (W1-->2)                     0               0
Processes (P1-->2)                       0            -100
SUM OF ALL TERMS                       100            -100
```

Waste loads plus inflow balanced by outflow of mass (steady state):

```
============================================================
Mass balances for segment X
============================================================
Substance Y                    Sources/Inflows Sinks/Outflows
------------------------------------------------------------
Storage  (M(t1) - M(t2))                 0               0
Transport (T1-->2)                      20            -120
Waste loads (W1-->2)                   100               0
Processes (P1-->2)                       0               0
SUM OF ALL TERMS                       120            -120
```

Waste loads balanced by outflow of mass, tidal conditions (dynamic equilibrium):

```
============================================================
Mass balances for segment X
============================================================
Substance Y                    Sources/Inflows Sinks/Outflows
------------------------------------------------------------
Storage  (M(t1) - M(t2))                 0               0
Transport (T1-->2)                    5000           -5100
Waste loads (W1-->2)                   100               0
Processes (P1-->2)                       0               0
SUM OF ALL TERMS                      5100           -5100
```

2 Implementation in Deltares software

2.1 General

In this paragraph we discuss how the mass balances feature is implemented in DELWAQ (DELWAQ is the programme carrying out the water quality calculations in both SOBEK and Delft3D). First we discuss the general aspects, followed by an explanation of aspects typical for SOBEK and Delft3D.

2.1.1 Types of output

DELWAQ provides two types of mass balance output:

1. Mass balances output integrated over the complete specified output period, in an ASCII file <∗-bal.prn>.
2. Mass balances output distributed over the specified intervals during the output period, in a DELWAQ binary history file <∗.his>.

The examples in this document only show the integrated ASCII output. Except the considerations under “time management” below, all explanations in this document apply for both types of output.

2.1.2 Time management

The time management of the mass balances output is linked to the monitoring output timers (which also decide the time management in the <∗.mon> file and the times written to the screen).

The period for the mass balances output is also echoed at the top of the ASCII output file (relative to the reference time, which is also listed):

```
Simulation starts: T0: 1976.01.01 00:00:00  (SCU=       1s)
Mass balances output period:
start:     0.000 days
stop : 21900.000 days
```

KNOWN BUGS:

1. Stop time of simulation should exactly match an output time for the ASCII output to be created.
2. Time period listed in ASCII file is the output period, which is not correct, if the output period is not within the simulation period.

2.1.3 Spatial definition (output areas)

The mass balances are constructed for the monitoring areas, which also form the basis for the “history” output of DELWAQ.

```
============================================================
Mass balances for Nuldernauw
============================================================
```

The mass balances are furthermore composed for the sum of all monitoring areas.

```
============================================================
Mass balances for Sum_of_balance_areas
============================================================
```

Optionally, the output for individual monitoring areas can be suppressed so that only the balance for the sum of all areas remains. A monitoring point or area can be excluded from the balance output by adding the keyword `NO_BALANCE` directly after the name of the monitoring point or area in the DELWAQ input file.

2.1.4 State variables

The mass balances are provided for all state variables of DELWAQ individually:

```
Substance OXY                 Sources/Inflows Sinks/Outflows
------------------------------------------------------------
...
Substance NH4                 Sources/Inflows Sinks/Outflows
------------------------------------------------------------
...
```

The mass balances are also provided for the total nitrogen (“TotN”) and phosphorus (“TotP”) mass in the water column:

```
Substance TotN                Sources/Inflows Sinks/Outflows
------------------------------------------------------------
...
Substance TotP                Sources/Inflows Sinks/Outflows
------------------------------------------------------------
...
```

The mass balances for total N and total P are the sum of the mass balances for those individual state variables that contain N and P, scaled with a stoichiometric constant expressing their relative N and P content (gN/g, gP/g). The actual composition of total N and P is listed at the top of the ASCII output file:

```
Balance for sum parameter TotN                consists of:
substance           scale factor
NH4                       1.0000
NO3                       1.0000
OON                       1.0000
DETN                      1.0000
FDIATOMS_E                0.2100
FDIATOMS_N                0.2000
GREENS_E                  0.2750
GREENS_N                  0.1750
GREENS_P                  0.2000
BLUEGRN_E                 0.2250
BLUEGRN_N                 0.1250
BLUEGRN_P                 0.1500
```

```
Balance for sum parameter TotP                consists of:
substance           scale factor
PO4                     1.0000
PAP                     1.0000
AAP                     1.0000
OOP                     1.0000
DETP                    1.0000
FDIATOMS_E              0.0180
FDIATOMS_N              0.0113
GREENS_E                0.0237
GREENS_N                0.0150
GREENS_P                0.0125
BLUEGRN_E               0.0188
BLUEGRN_N               0.0137
BLUEGRN_P               0.0113
```

Note: that the selected algae species are represented in this balance with the correct stoichiometric ratios (gN/gC, gP/gC).

2.1.5 Units

The balances are calculated in "basic mass units". If the Processes Library is used, this unit is [g] by definition. If the Processes Library is not used, this unit is not fixed and implicitly determined by the units used in the DELWAQ input files (for boundary conditions and waste loads).

The balances in the $<*$.his$>$ file are written in [g], [g/m^2] or [g/m^3]. The ASCII output files presents the balances in all three units, as indicated in the file:

```
MASS BALANCE PER DUMPAREA
All terms in basic mass units,for Processes Library always [g]
......
MASS BALANCE PER SURFACE
All terms in basic mass units/m2,for Processes Library always [g]
...
MASS BALANCE PER VOLUME
All terms in basic mass units/m3,for Processes Library always [g]
```

TODO(??): *To be included: precise specification of surface and volume used to scale mass balances.* **TODO**

Warning: we advise to use mass balances in mass units only, because this allows for unambiguous interpretation.

TODO(??): *To be included: how to define units in time dependent output.* **TODO**

2.1.6 Definition of transport terms

The transport terms are separated in two parts.

1 Transport over model boundaries, either as a total, or subdivided over the different types or clusters of model boundaries.

Substance NO3	Sources/Inflows	Sinks/Outflows
NO3 _Storage	0.57888E+07	0.00000E+00
NO3 _All Bo+Lo	**0.68367E+08**	**-0.54284E+07**
NO3 _Internal transport	0.27253E+08	-0.12143E+08
NO3 _dNO3Upt	0.00000E+00	-0.98418E+08
NO3 _dDenitWat	0.00000E+00	0.00000E+00
NO3 _dNitrif	0.33922E+07	0.00000E+00
NO3 _dNO3UptS1	0.00000E+00	-0.32777E-07
NO3 _MSN0DI	0.11189E+08	0.00000E+00
SUM OF ALL TERMS	0.11599E+09	-0.11599E+09

Substance AAP	Sources/Inflows	Sinks/Outflows
AAP _Storage	0.00000E+00	-0.64501E+09
AAP _Diffuse l	**0.61687E+09**	**0.00000E+00**
AAP _Upstream	**0.59562E+10**	**0.00000E+00**
AAP _Normal la	**0.39978E+09**	**0.00000E+00**
AAP _Sea Bound	**0.00000E+00**	**-0.81145E+10**
AAP _Loads	0.00000E+00	0.00000E+00
AAP _Internal transport	0.17756E+12	-0.17756E+12
AAP _Processes	0.17888E+10	0.00000E+00
SUM OF ALL TERMS	0.18632E+12	-0.18632E+12

Note: that in the “lumped” mode, the transport over the model boundaries is also lumped with the waste loads (“_All Bo+Lo”).

1 Transport to and from other areas inside the model area, (internal transport) either as a total or subdivided over the transport to and from the other monitoring areas and the transport to and from the remaining model area.

Substance NO3	Sources/Inflows	Sinks/Outflows
NO3 _Storage	0.57888E+07	0.00000E+00
NO3 _All Bo+Lo	0.68367E+08	-0.54284E+07
NO3 _Internal transport	**0.27253E+08**	**-0.12143E+08**
NO3 _dNO3Upt	0.00000E+00	-0.98418E+08
NO3 _dDenitWat	0.00000E+00	0.00000E+00
NO3 _dNitrif	0.33922E+07	0.00000E+00
NO3 _dNO3UptS1	0.00000E+00	-0.32777E-07
NO3 _MSN0DI	0.11189E+08	0.00000E+00
SUM OF ALL TERMS	0.11599E+09	-0.11599E+09

Substance Total	Sources/Inflows	Sinks/Outflows
Total _Storage	0.00000E+00	-0.17092E+09
Total _All Bo+Lo	0.11950E+13	-0.12031E+13
Total _Other	**0.00000E+00**	**0.00000E+00**
Total _Overall	**0.00000E+00**	**0.00000E+00**

Total _ZWKust01	**0.00000E+00**	**-0.64929E+10**
Total _ZWKust12	**0.34305E+11**	**-0.60816E+11**
Total _NDKust01	**0.00000E+00**	**0.00000E+00**
Total _NDKust12	**0.84880E+10**	**-0.51898E+10**
Total _HollKust0	**0.00000E+00**	**0.00000E+00**
Total _HollKust1	**0.18322E+11**	**-0.41308E+11**
Total _Wadkust01	**0.00000E+00**	**0.00000E+00**
Total _Wadkust12	**0.19543E+12**	**-0.18836E+12**
Total _EemsKust	**0.67386E+11**	**-0.22286E+11**
Total _EDolKust	**0.97467E+10**	**-0.77715E+09**
Total _EDollard	**0.00000E+00**	**0.00000E+00**
Total _WestSchel	**0.00000E+00**	**0.00000E+00**
Total _Waddenzee	**0.00000E+00**	**0.00000E+00**
Total _OostSchel	**0.00000E+00**	**0.00000E+00**
Total _Processes	0.00000E+00	0.00000E+00
SUM OF ALL TERMS	0.15287E+13	-0.15285E+13

Note: that the first internal transport term (if not lumped) is denoted "_Other".

2.1.7 Definition of waste load term

The waste load terms are either lumped with the transport over the open model boundaries, or separately listed, subdivided over the different types or classes of waste loads.

Substance NO3	Sources/Inflows	Sinks/Outflows
NO3 _Storage	0.57888E+07	0.00000E+00
NO3 _All Bo+Lo	**0.68367E+08**	**-0.54284E+07**
NO3 _Internal transport	0.27253E+08	-0.12143E+08
NO3 _dNO3Upt	0.00000E+00	-0.98418E+08
NO3 _dDenitWat	0.00000E+00	0.00000E+00
NO3 _dNitrif	0.33922E+07	0.00000E+00
NO3 _dNO3UptS1	0.00000E+00	-0.32777E-07
NO3 _MSN0DI	0.11189E+08	0.00000E+00
SUM OF ALL TERMS	0.11599E+09	-0.11599E+09

Substance NO3	Sources/Inflows	Sinks/Outflows
NO3 _Storage	0.70697E+05	0.00000E+00
...		
NO3 _deep-sedi	0.00000E+00	0.00000E+00
NO3 _C_P1_129	**0.23518E+06**	**-0.17312E+02**
NO3 _C_P1_101	**0.19132E+06**	**-0.23944E+02**
...		
NO3 _wash_sr1	**0.00000E+00**	**0.00000E+00**
NO3 _sewer_sr1	**0.18360E+07**	**0.00000E+00**
NO3 _Other	0.00000E+00	0.00000E+00
NO3 _water	0.00000E+00	0.00000E+00
NO3 _sediment	0.29136E+08	-0.16680E+08
NO3 _dNO3Upt	0.00000E+00	-0.10100E+09
...		
NO3 _dAtmDepNO3	0.33704E+07	0.00000E+00
SUM OF ALL TERMS	0.12652E+09	-0.12652E+09

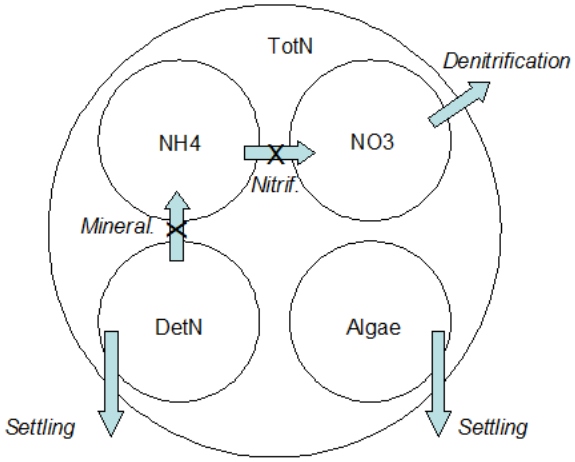
2.1.8 Definition of processes term

The processes term is either provided as a total, or subdivided over individual processes.

Substance AAP		Sources/Inflows	Sinks/Outflows
AAP	_Storage	0.00000E+00	-0.64501E+09
AAP	_Diffuse l	0.61687E+09	0.00000E+00
AAP	_Upstream	0.59562E+10	0.00000E+00
AAP	_Normal la	0.39978E+09	0.00000E+00
AAP	_Sea Bound	0.00000E+00	-0.81145E+10
AAP	_Loads	0.00000E+00	0.00000E+00
AAP	_Internal transport	0.17756E+12	-0.17756E+12
AAP	**_Processes**	**0.17888E+10**	**0.00000E+00**
SUM OF ALL TERMS		0.18632E+12	-0.18632E+12

Substance NO3		Sources/Inflows	Sinks/Outflows
NO3	_Storage	0.57888E+07	0.00000E+00
NO3	_All Bo+Lo	0.68367E+08	-0.54284E+07
NO3	_Internal transport	0.27253E+08	-0.12143E+08
NO3	**_dNO3Upt**	**0.00000E+00**	**-0.98418E+08**
NO3	**_dDenitWat**	**0.00000E+00**	**0.00000E+00**
NO3	**_dNitrif**	**0.33922E+07**	**0.00000E+00**
NO3	**_dNO3UptS1**	**0.00000E+00**	**-0.32777E-07**
NO3	**_MSN0DI**	**0.11189E+08**	**0.00000E+00**
SUM OF ALL TERMS		0.11599E+09	-0.11599E+09

For the balances consisting of more than one state variable (total N and P), the processes which transform one state variable inside the balance to another state variable inside the balance are not included in the balance. For example, in a balance for total N, the processes nitrification and mineralization do not appear, while processes like settling of detritus N or algae and denitrification do appear, see the figure below.



2.1.9 Gross and net terms

The transport terms show both positive (inflow) and negative (outflow) terms, so that the gross and the net transport are provided.

There is one exception though. In cases where simultaneous inflows and outflows are taking place via different boundaries connected to the same monitoring area, the mass balances will include only the net transport. **TODO(??):** *to be confirmed*

TODO

The processes terms for individual processes are with few exceptions by definition either always negative or always positive. If the processes are lumped to one term, only the net result is provided, either as a positive or as a negative term.

2.1.10 Customising the mass balances output

The configuration of the mass balances can be controlled by the user, by means of certain switches. The intention of these switches is to allow the user to avoid unnecessarily large output files. The control options are:

- ◇ To suppress the time dependent balances output in the .HIS file.
- ◇ To suppress output for individual monitoring areas (only output for sum of areas).
- ◇ To lump processes terms.
- ◇ To lump boundary and load terms,
- ◇ To lump internal transport terms.

The User Interfaces of SOBEK and Delft3D allow the user to manipulate the switches. Users of SOBEK and Delft3D can skip the remainder of this section.

The stand-alone user can control these switches either by keywords in the input file or in a special <delwaq.ini> file which needs to be present on the directory where DELWAQ is running. The keywords in the input file follow after the definition of the computational scheme:

```
   5.73   ; integration option
   BAL\_NOLUMPPROCESSES BAL\_LUMPLOADS BAL\_NOLUMPTRANSPORT
   BAL\_NOSUPPRESSSPACE BAL\_SUPPRESSTIME  ; .prn mass balance output

;        dddhhmmss
0      ; start time
365000000      ; stop time
0      ; constant timestep
0003000      ; time step
```

The relevant section of the delwaq.ini file looks as follows:

```
[Balance Options]
LumpProcessesContributions=0
LumpBoundaryContributions=-1
SumOfMonitoringAreas=0
SuppressTimeDependentOutput=0
```

The table below provides the options and their definition in the input file and in the <delwaq.ini> file.

Table 2.1: *Options*

Description of flag	**Value**	**Definition in input**	**Definition in <delwaq.ini>**
Option to suppress time dependent balances output	Active	BAL_SUPPRESSTIME	SuppressTimeDependentOutput=-1
	Inactive	BAL_NOSUPPRESSTIME	SuppressTimeDependentOutput=0
Option to suppress space dependent output	Active	BAL_SUPPRESSSPACE	SumOfMonitoringAreas=-1
	Inactive	BAL_NOSUPPRESSSPACE	SumOfMonitoringAreas=0

Option to lump processes terms	Active Inactive	BAL_LUMPPROCESSES BAL_NOLUMPPROCESSES	LumpProcessesContributions=-1 LumpProcessesContributions=0
Option to lump loads and boundaries terms	Active Inactive	BAL_LUMPLOADS BAL_NOLUMPLOADS	LumpBoundaryContributions=-1 LumpBoundaryContributions=0
Option to lump internal transport terms	Active Inactive	BAL_LUMPTRANSPORT BAL_NOLUMPTRANSPORT	LumpInternalTransport=-1 vLumpInternalTransport=0

2.2 Specific SOBEK aspects

This part is specific for the SOBEK UI. It will describe how the balance output can be switched on and how different options are set. Basic understanding of the SOBEK UI is needed or can be found in the SOBEK manual.

2.2.1 Task block Settings

In this part the basic settings for the balance options are set. For the balance options two main tab forms are important.

2.2.1.0.1 Output Options

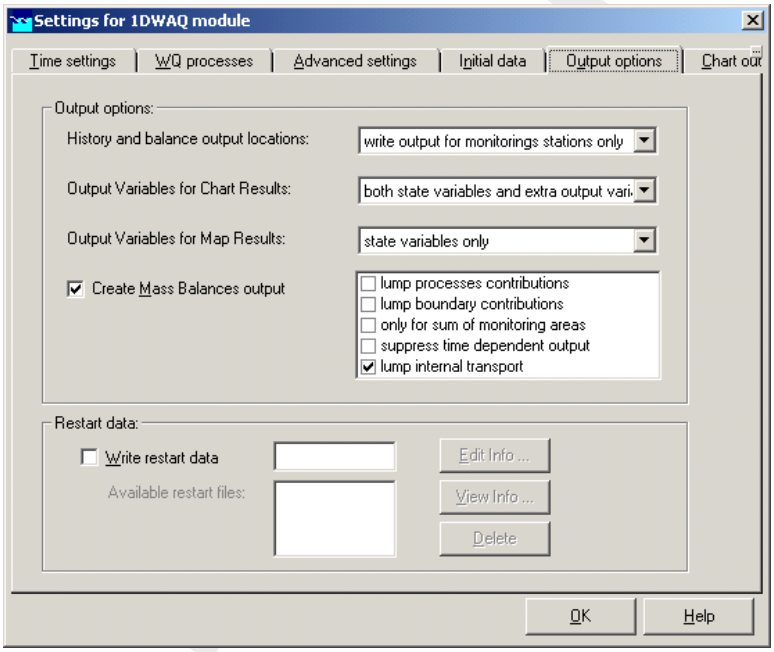


Figure 2.1: *Settings for 1DWAQ module; output options*

In this tab form the user can specify all basic Balance settings. Balances can be created for every Delwaq segment or only for monitoring stations. These are specified locations in the SOBEK network.

2.2.1.0.2 Balance Output

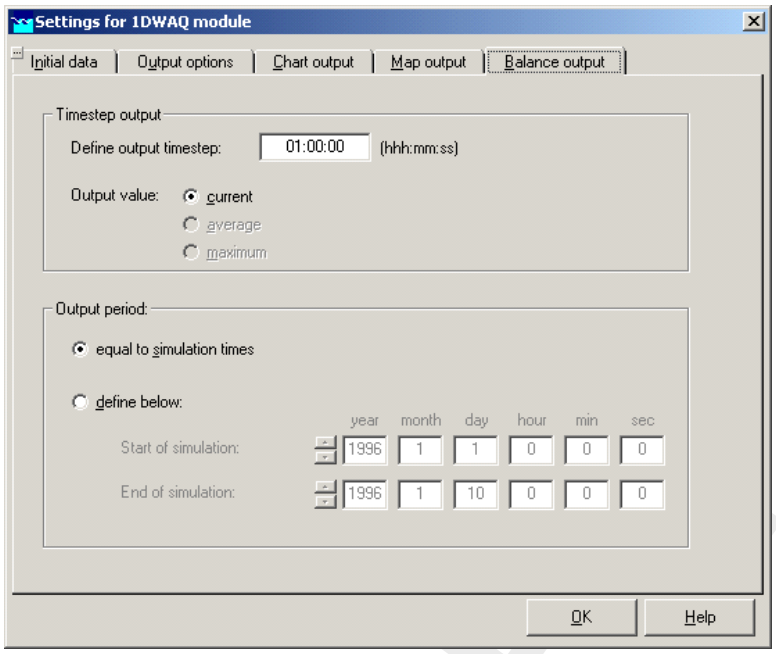


Figure 2.2: *Settings for 1DWAQ module; balance output*

On this tab form the user can specify a specific output period and time step for the mass balances.

Note: See “Known bugs” in subsection 2.1.2.

2.2.2 Schematisation and monitoring areas

In this part the user can specify the monitoring areas and specific output locations in SOBEK.

To create output for area’s the user should specify a “Surface Water Type” and link it to a channel flow object in SOBEK. Basically, the user clones a “branch object” to create a special area. This can be done in the “Edit User Defined Objects” menu in the Schematisation task block.

2.2.2.0.1 Edit User Defined Objects

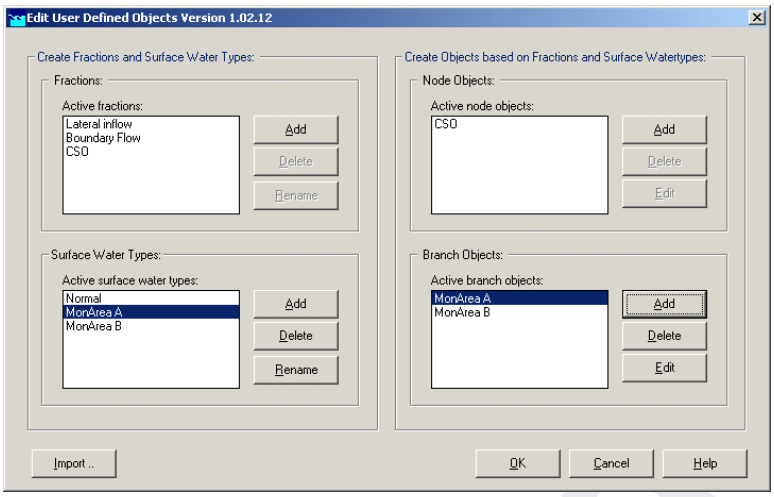


Figure 2.3: *User defined Objects*

A “surface water type” (SWT) is a special type of water where a user can specify local process coefficients, dispersion and initial conditions. Based on the SWT also a monitoring area is defined. In the menu screen a user should first create a SWT and then link it to a new “branch object”. Use as parent type a Flow – Channel object. In the SOBEK manual more information can be found on the User Defined objects.

Note: Please create for every unique SWT also a unique branch object!

2.2.2.0.2 Edit model (Netter)

The newly created branch objects can be found in Netter.

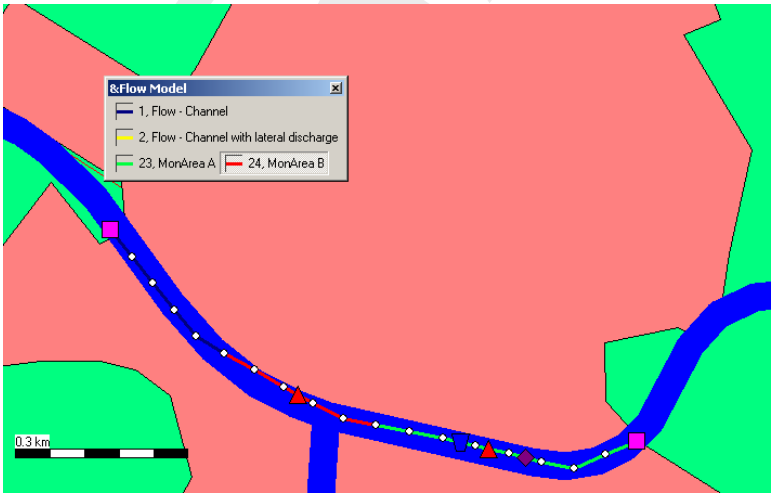


Figure 2.4: *Flow model*

Now they can be used in the same way the normal Flow – Channel branches could be used.

Note: also the Flow – Measurement stations (red triangles). On these locations the Delwaq history output will be available.

2.2.3 Output

Every SWT counts as a monitoring area. On every monitoring area balance output can be found. A balance area starts with a prefix “SWT_”. The ASCII balance output can be found in the “Results in tables” task block. The time dependent balance output file can be found in the “Results in charts” task block.

2.2.3.1 Results in tables

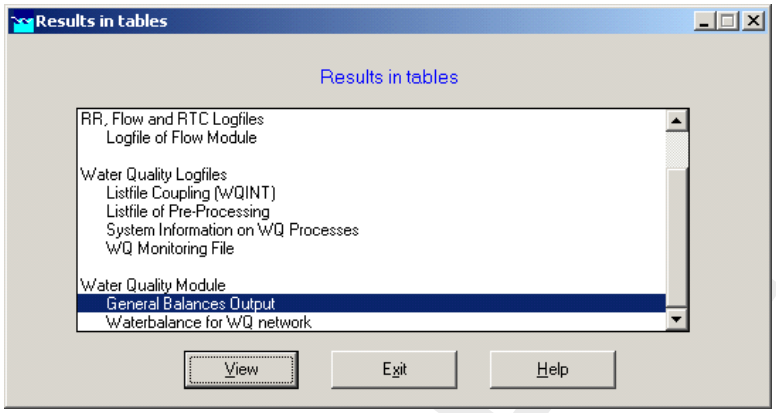


Figure 2.5: *Result in tables*

For a certain Monitoring Area the ASCII balance will look like:

```
...
============================================================
Mass balances for SWT_MonAreaA
============================================================
Substance NH4                    Sources/Inflows Sinks/Outflows
------------------------------------------------------------
NH4   _Storage                     0.88805E+02    0.00000E+00
NH4   _Boundary                    0.77760E+04    0.00000E+00
NH4   _CSO                         0.59400E+04    0.00000E+00
NH4   _Loads                       0.00000E+00    0.00000E+00
NH4   _Internal transport          0.00000E+00   -0.12906E+05
NH4   _dNitrif                     0.00000E+00   -0.89938E+03
NH4   _dTEWORNH4                   0.00000E+00    0.00000E+00
SUM OF ALL TERMS                   0.13805E+05   -0.13805E+05
...
```

The “Sum_of_balance_areas” is also given in the ASCII balance output. This option can be useful to analyse the balance of all balance areas. But be careful using this option. Sometimes a Delwaq segment is used in multiple monitoring area’s, for example as specific location and in a Surface Water Type. Then the segment is counted **twice** in the Sum_of_balance_areas output.

```
...
============================================================
Mass balances for Sum_of_balance_areas
============================================================
Substance NH4                    Sources/Inflows Sinks/Outflows
------------------------------------------------------------
```

```
NH4    _Storage                    0.44628E+03     0.00000E+00
...
```

2.2.3.2 Results in Charts

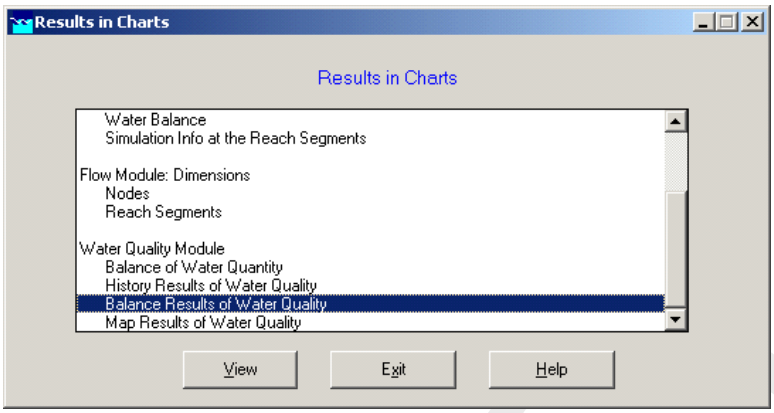


Figure 2.6: *Result in charts*

In results in charts a His file with balance output will be available.

Note: The history file for balances output in SOBEK is always in the unit mass per output time step.

2.2.4 Special remarks

The SOBEK UI uses the <delwaq.ini> file for triggering the balances. It is also possible to "hack" the keywords directly into the Delwaq input file, but then the UI will be crashing later on.

TODO **TODO(??):** *In the latest SOBEK version (May 2008) the detailed internal transport option is not available yet. This will be implemented in Delwaq (SOBEK) soon (Jira SOBEK-19744). Ask Erwin Meijers for the exact status or check Jira.*

2.2.5 WQint

WQint is the coupling program for SOBEK. When creating monitoring areas WQint will provide the Delwaq segment numbers for every monitoring area. In august 2007 some major adjustments are made to WQint to write monitoring area's per surface water type.

In the <wqint.ini> file (<SOBEK\Programs\Delwaq>) three switches are implemented:

Table 2.2: *Switches*

Switch or flag	Value	Result
UseMonStatWQ	-1 0	Use <monstat.wq> file is used for defining monitoring areas (old default). Do not use <monstat.wq> file (current default)
UseMeasStats	-1 0	Monitoring stations are applied for node type: Flow – Measurement Station (default) No use of Measurement stations

UseRestMonArea	-1 0	Use Monitoring Area for every Surface Water Type (default) No use of SWT

2.3 Specific Delft3D aspects

The options for the mass balances are specified under “Output Options”, select “Extended Mass Balances”. The options are easily understood on the basis of the descriptions in section 2.1.

The monitoring areas you need for creating useful mass balances, need to be imported in the WAQ-GUI from an external file $<*$.dmo$>$. This file can be made with the DIDO program.

Note: Monitoring points and monitoring areas can interfere with each other if monitoring points are located at the edges of the areas. See subsection 2.1.3 for details on how to switch off balances output for monitoring points.

3 Examples of presentation techniques

3.1 Methodology

All presentation formats presented herein are prepared in Excel, on the basis of the ASCII balances output file, which covers the total output period. The following procedure is followed:

- ◇ The output file is copied to one sheet of the Excel file (the “data” sheet).
- ◇ The presentation sheet selects its value from the data sheet.
- ◇ As long as the model configuration and the selected options of the mass balances do not change, the format of the balances output will remain unchanged, and the presentation can be updated for new model runs by simply copying the new balance file to the data sheet.

In a similar fashion parts of the time dependent mass balances file can be used, for example by exporting the relevant data with the ODS_View tool to Excel, or by importing time dependent mass balances in MatLab. This will not be further discussed.

3.2 Examples

3.2.1 Overal system balance for Pungol-Serangoon reservoir

3.2.2 Fluxes between and transformations inside “boxes” (North Sea priority pollutants)

3.2.3 Elaborate water and nutrient balances for subdivided system (Southern Delta – The Netherlands)

4 Interpretation and detection of errors

This chapter discusses only the time-integrated balance output file. Similar considerations are valid for the time-dependent balances output.

4.1 Mass errors in the balances

The mass balances are presented in two columns, one holding the positive and the other holding the negative terms. The sum of all numbers in both columns is provided, for easy checking. What to do if the sum of both columns is not consistent?

```
Sources/Inflows Sinks/Outflows
SUM OF ALL TERMS                  0.55347E+13   -0.55344E+13
```

1 Small discrepancies can occur due to the fact that DELWAQ calculates in single precision (4 bytes reals). This implies that if calculus is done with numbers differing several orders of magnitude, inaccuracies may arise. This happens for instance:

   1.1 Over tidal boundaries, where the gross transport terms in the mass balance are several orders of magnitude larger than any of the other balance terms.
   1.2 In the sediment, where the pools and the fluxes may differ several orders of magnitude, and a mismatch between both can be created.

   Generally speaking, this type of discrepancies can be neglected as long as it does not affect the balance in the form you present it (if the error becomes invisible when you round the numbers).

2 Discrepancies arise if the so-called “closure error correction” is active. This is a feature of DELWAQ that may be used when a hydrodynamic file is rewound, and a discontinuity is created in the water volumes. Because DELWAQ is mass conserving, this results in a discontinuity in the concentrations. The “closure error correction” avoids this by deliberately creating a discontinuity in the mass. Because there is no equivalent flux, this leads to a discrepancy in the mass balances. The “closure error correction” is standard in Delft3D.

```
Sources/Inflows Sinks/Outflows
SUM OF ALL TERMS                  0.45637E+08   -0.52984E+01
```

3 Extreme errors like in the example above can be the result of a simulation with numerical methods 15/16 if the water quality processes cause instabilities. Sometimes the simulation does not crash (Linux!!), but yields very strange results, which also lead to large errors in the mass balances. Such problems are known to occur for example:

   3.1 If very shallow segments are present which are not made inactive;
   3.2 If the water volume of a discharge has been erroneously neglected in the hydrodynamics, and at the same time substance loads of for example Oxy (8 mg/l), Temp (20 °C) etc. are defined.

4 If you have a significant mass error and neither of the explanations above applies: contact your nearest DELWAQ dealer!

4.2 Check on missing and/or unwanted processes

If you create a mass balances output file with all individual processes, you can see:

◇ which processes are activated (because they occur in the mass balances);
◇ which processes have a flux equal to zero and which processes not.

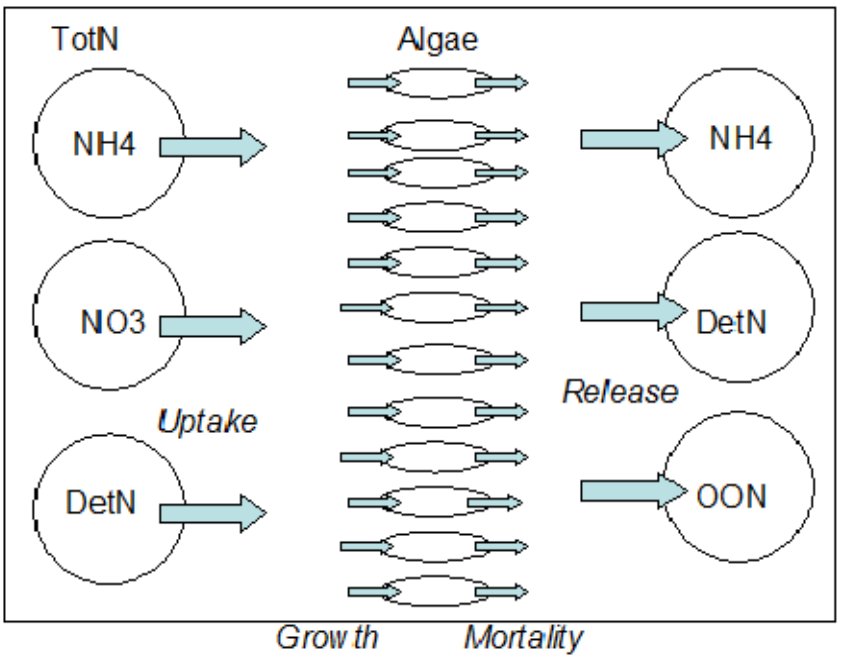
The occurrence of unexpected processes, or the lacking of expected processes, or a flux of zero for certain processes where you did not deliberately make a rate constant zero are all indications that the model input may not be entirely correct. A check like this is quickly made and may save you a lot of headaches later on.

4.3 Algae balance

The algae balances in DELWAQ need special attention.

- ◇ DELWAQ does not provide a balance for total carbon, nor for carbon in algae.
- ◇ DELWAQ only provides balances for individual algae types.
- ◇ Unfortunately, DELWAQ is not able to omit the fluxes related to the uptake and release of N and P by algae from the N and P balances. Such fluxes should be omitted because they represent transformations from one pool of N or P inside the balance to another pool of N and P inside the balance.

The explanation for the latter issue is provided by the figure below.



DELWAQ mass balances can only correctly omit fluxes from composite mass balances if these fluxes are defined “from” one state variable “to” another, both inside the mass balance. The uptake and release of nutrients by algae do not satisfy that condition. For nitrogen, the uptake is defined as a sink for NH4, NO3 and DetN. The growth is defined as individual source fluxes for every algae type. The mortality is defined as individual sink fluxes for every algae type. The release of nutrients is defined as a source of NH4, detritus and other organic matter.

Consequently, all fluxes shown in the picture show up in the total N and P balances. The consistency of these fluxes is not controlled by DELWAQ adding and subtracting all processes fluxes, but by the underlying process which calculates all these fluxes. In the recent past we have had some surprises in this respect. Therefore, we advise the users to validate that the sum of all the fluxes in the picture above is indeed correct. The example below shows which fluxes this concerns.

Substance TotN	Sources/Inflows	Sinks/Outflows
TotN _Storage	0.10238E+08	0.00000E+00
TotN _All Bo+Lo	0.17849E+09	-0.12256E+09
TotN _Internal transport	0.27085E+09	-0.29250E+09
TotN _dNaut	**0.19064E+09**	**0.00000E+00**
TotN _dDetNMort	**0.39712E+09**	**0.00000E+00**
TotN _dOONMort	**0.49151E+08**	**0.00000E+00**
TotN _dNH4Upt	**0.00000E+00**	**-0.66795E+09**
TotN _dNO3Upt	**0.00000E+00**	**-0.98418E+08**
TotN _dDetNUpt	**0.00000E+00**	**0.00000E+00**
TotN _dProdAlg01	**0.28518E+08**	**0.00000E+00**
TotN _dProdAlg02	**0.45352E+07**	**0.00000E+00**
TotN _dProdAlg03	**0.29314E+06**	**0.00000E+00**
TotN _dProdAlg04	**0.57122E+08**	**0.00000E+00**
TotN _dProdAlg05	**0.31359E+08**	**0.00000E+00**
TotN _dProdAlg06	**0.11823E+09**	**0.00000E+00**
TotN _dProdAlg07	**0.11663E+09**	**0.00000E+00**
TotN _dProdAlg08	**0.40828E+09**	**0.00000E+00**
TotN _dMortAlg01	**0.00000E+00**	**-0.23318E+08**
TotN _dMortAlg02	**0.00000E+00**	**-0.64222E+07**
TotN _dMortAlg03	**0.00000E+00**	**-0.10582E+06**
TotN _dMortAlg04	**0.00000E+00**	**-0.28739E+08**
TotN _dMortAlg05	**0.00000E+00**	**-0.57732E+08**
TotN _dMortAlg06	**0.00000E+00**	**-0.61869E+08**
TotN _dMortAlg07	**0.00000E+00**	**-0.59573E+08**
TotN _dMortAlg08	**0.00000E+00**	**-0.39916E+09**
TotN _dDenitWat	0.00000E+00	0.00000E+00
TotN _dMinDetNS1	0.00000E+00	0.00000E+00
TotN _dNH4UptS1	0.00000E+00	-0.10461E+05
TotN _dNO3UptS1	0.00000E+00	-0.32777E-07
TotN _dNH4US1D	0.00000E+00	0.00000E+00
TotN _dNH4AUTS1	0.00000E+00	0.00000E+00
TotN _dSedDetN	0.00000E+00	-0.76079E+08
TotN _dSedOON	0.00000E+00	-0.28184E+08
TotN _dSWSedOON	0.00000E+00	0.00000E+00
TotN _dSedAlg01	0.00000E+00	0.00000E+00
TotN _dSedAlg02	0.00000E+00	0.00000E+00
TotN _dSedAlg03	0.00000E+00	0.00000E+00
TotN _dSedAlg04	0.00000E+00	0.00000E+00
TotN _dSedAlg05	0.00000E+00	0.00000E+00
TotN _dSedAlg06	0.00000E+00	0.00000E+00
TotN _dSedAlg07	0.00000E+00	0.00000E+00
TotN _dSedAlg08	0.00000E+00	0.00000E+00
TotN _dResS1DetN	0.16170E+08	0.00000E+00
TotN _dResS2DetN	0.00000E+00	0.00000E+00
TotN _dResS1DiDN	0.43413E+04	0.00000E+00
TotN _dGrzDisN	0.14565E+07	0.00000E+00
TotN _dGrzDetN	0.68318E+07	0.00000E+00
TotN _dGrzALG01	0.00000E+00	-0.10909E+06
TotN _dGrzALG02	0.00000E+00	-0.21362E+05
TotN _dGrzALG03	0.00000E+00	-0.60031E+03
TotN _dGrzALG04	0.00000E+00	-0.36290E+06
TotN _dGrzALG05	0.00000E+00	-0.22798E+06
TotN _dGrzALG06	0.00000E+00	-0.68573E+06
TotN _dGrzALG07	0.00000E+00	-0.12505E+07
TotN _dGrzALG08	0.00000E+00	-0.94311E+07
TotN _MSA0DI	0.37601E+08	0.00000E+00
TotN _MSA0Z	0.00000E+00	0.00000E+00
TotN _MSN0DI	0.11189E+08	0.00000E+00
SUM OF ALL TERMS	0.19347E+10	-0.19347E+10

The sum of all these fluxes should normally be zero (rounded). The only exception is the

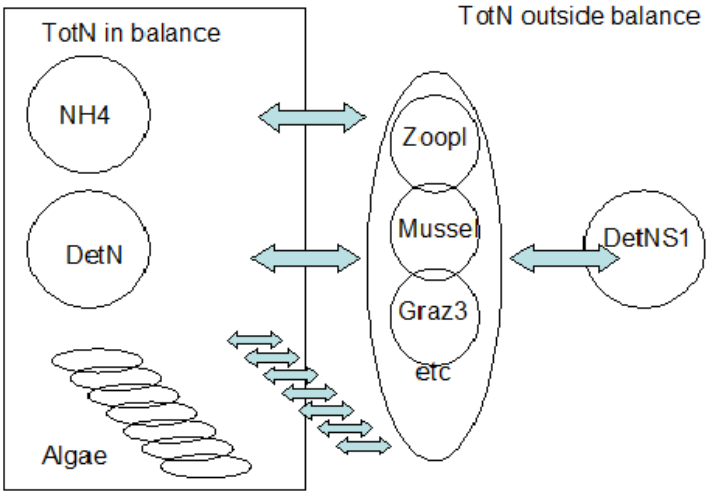
presence of N-fixating algae in the model. This will cause the sum of the relevant terms in the N balance to be >0 (production of N in algae without the corresponding negative uptake flux).

4.4 Sediment balance

DELWAQ does not produce an overall balance for the sediment, neither does it produce a balance for the total of the water column and the sediment. Therefore, it is left to the user to derive a sediment balance and to check the consistency between both balances. If a simple sediment model is used, such checks are trivial and easy. However, if more complex sediment approaches are used, such as Switch, Delwaq-G, bottom algae etc., we strongly advise to check the sediment balances and the interactions between the sediment and the water.

4.5 Consumers balance (grazing)

Another non-trivial issue in the mass balances is the balance of grazers, if these are represented by the CONSBL process. CONSBL does not create state variables for the grazers, and therefore there is a “hole” in the total N and total P balance, see the figure.



The picture is further complicated because the grazers optionally excrete detritus to the sediment (DetNS1 in the figure) which implies a flux from the water column to the sediment like in the case of sedimentation.

In the recent past there have been problems related to CONSBL. Therefore, we strongly recommend to calculate the sum of all fluxes related to CONSBL and verify that this sum is correct. The example below shows which fluxes this concerns.

```
Substance TotN                  Sources/Inflows Sinks/Outflows
-------------------------------------------------------------
TotN  _Storage                     0.10238E+08    0.00000E+00
TotN  _All Bo+Lo                   0.17849E+09   -0.12256E+09
TotN  _Internal transport          0.27085E+09   -0.29250E+09
TotN  _dNaut                       0.19064E+09    0.00000E+00
...
TotN  _dResS1DiDN                  0.43413E+04    0.00000E+00
TotN  _dGrzDisN                    0.14565E+07    0.00000E+00
```

TotN	**_dGrzDetN**	**0.68318E+07**	**0.00000E+00**
TotN	**_dGrzALG01**	**0.00000E+00**	**-0.10909E+06**
TotN	**_dGrzALG02**	**0.00000E+00**	**-0.21362E+05**
TotN	**_dGrzALG03**	**0.00000E+00**	**-0.60031E+03**
TotN	**_dGrzALG04**	**0.00000E+00**	**-0.36290E+06**
TotN	**_dGrzALG05**	**0.00000E+00**	**-0.22798E+06**
TotN	**_dGrzALG06**	**0.00000E+00**	**-0.68573E+06**
TotN	**_dGrzALG07**	**0.00000E+00**	**-0.12505E+07**
TotN	**_dGrzALG08**	**0.00000E+00**	**-0.94311E+07**
TotN	_MSA0DI	0.37601E+08	0.00000E+00
TotN	_MSA0Z	0.00000E+00	0.00000E+00
TotN	_MSN0DI	0.11189E+08	0.00000E+00
SUM OF ALL TERMS		0.19347E+10	-0.19347E+10

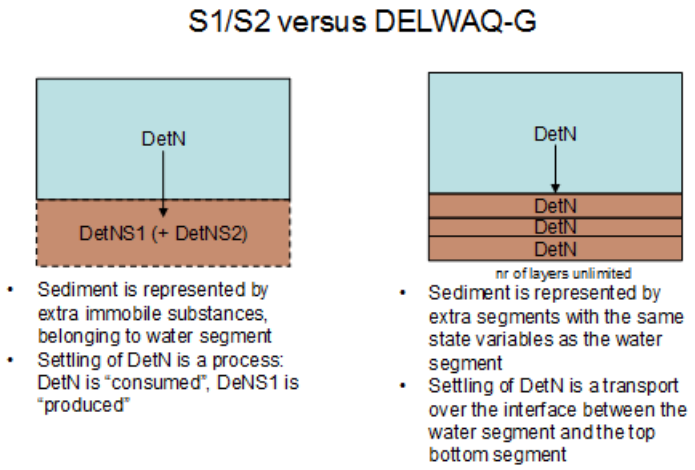
Substance DetNS1	Sources/Inflows	Sinks/Outflows
DetNS1_Storage	0.87036E+05	0.00000E+00
DetNS1_All Bo+Lo	0.00000E+00	0.00000E+00
DetNS1_Internal transport	0.00000E+00	0.00000E+00
DetNS1_dMinDetNS1	0.00000E+00	0.00000E+00
DetNS1_dSWMinDNS1	0.00000E+00	-0.31473E+08
DetNS1_dMrtDetNS1	0.27897E+05	0.00000E+00
DetNS1_dSedDetN	0.76079E+08	0.00000E+00
DetNS1_dSedAlgN	0.00000E+00	0.00000E+00
DetNS1_dResS1DetN	0.00000E+00	-0.16170E+08
DetNS1_dBurS1DetN	0.00000E+00	0.00000E+00
DetNS1_dSWBuS1DtN	0.00000E+00	-0.32341E+08
DetNS1_dGrzDetNS1	**0.37898E+07**	**0.00000E+00**
SUM OF ALL TERMS	0.79983E+08	-0.79983E+08

The sum of all fluxes related to grazing should be zero, unless:

- ◇ There is a substantial increase or decrease of the grazers' biomass during the simulation. The associated storage or release of nutrients will result in a sum of all grazer related fluxes > 0 (grazer biomass decreases) or < 0 (grazer biomass increases). Evidently, this should also be checked quantitatively.
- ◇ The recently developed harvesting process is implemented. The associated removal of nutrients will result in a sum of all grazer related fluxes < 0. Again, this should also be checked quantitatively.

Note: that if there is a flux of nutrients from the grazers to the sediment, the sum of all grazer related fluxes in the total N (water) balance will be < 0. This is correct, it is an "enhanced settling" process induced by filtering mussels.

4.6 Sediment modelling: S1/S2 versus DELWAQ-G



In a traditional S1/S2 model, the sediment water exchange fluxes can be found as processes. In a DELWAQ-G model the sediment water exchange fluxes are internal transports.

While interpreting the internal transports at the sediment water interface in a DELWAQ-G application, please bear in mind:

- ◇ The sediment water exchange fluxes found in the total N and total P balances are the sum of:
  - downward fluxes of settling particulate substances (including settling algae);
  - optionally, upward fluxes of resuspending particulate substances;
  - diffuse exchange fluxes of dissolved substances.
- ◇ To break down the sediment water exchange fluxes in to these components, you have to look at the balances for individual substances:
  - for particular substances, the down term represents settling, the up term represents resuspension;
  - for dissolved substances, diffuse transport causes two terms of opposite sign, the actual diffusive flux is the net result of these two terms.
- ◇ The contributions of algae to the settling and resuspension fluxes of N and P has to be derived from the mass balances for the individual algae types (in gC), multiplied by the N:C and P:C ratios of the algae types respectively (as they are printed at the top of the $<*$-bal.prn$>$ file).

4.7 Exercises

4.7.1 Exercise 1

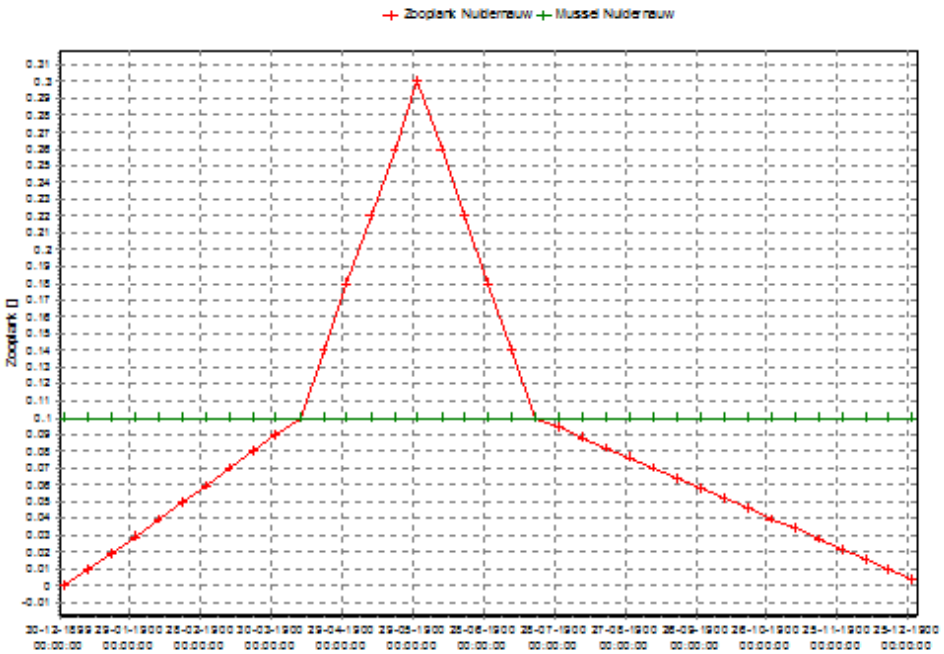
Check the balance file. Look at area Nuldernauw, start with balances for total N and P and use other balances whenever necessary.

1. Try to identify the algae related terms, see section 4.3. How many algae types are there?
2. Determine the algae balance. Is it consistent?
3. Check out the sign of the algae production terms. What do you see? Do you believe this?

TODO **TODO(??):** *Check with Hans Los*.

4. Is there any grazing?
5. Does it have a direct impact on the sediment?

6 Determine the grazer balance. Is it consistent (see graph of grazer biomass during simulation below)? This fits qualitatively with the observed small biomass increase of Zooplankton. Quantitative check needs to be done using change in biomass, stoichiometric ratio and segment volume!



7 Is the grazer induced flux of nutrients towards the sediment significant in view of the sedimentation fluxes towards the sediment?
8 Which fluxes do you recognise in the total N and total P balances from the water column towards the sediment?
9 Which fluxes do you recognise in the total N and total P balances from the sediment towards the water column?
10 Which other fluxes do you recognise?
11 Which unexpected/unknown processes have a flux not equal to zero?
12 Which processes have a zero flux? Is that a problem?

4.7.2 Exercises 2 to 5.

Look for anomalies . . .

4.7.3 Singapore exercise.

Take the balance file, select a state variable which shows interaction with the sediment, and make a mass balance picture as in the example shown during the course.

Photo by: Mathilde Matthijsse, www.zeelandonderwater.nl

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