

# MIKE 21 Flow Model

MIKE ECO Lab Module

**User Guide** 





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## 1 About This Guide

# 1.1 Purpose

The main purpose of this User Guide is to get you started in the use of MIKE 21 Flow Model ECO Lab Module, for applications involving ecological modelling. This User Guide is complemented by the Online Help.

# 1.2 Assumed User Background

Although the MIKE ECO Lab module has been designed carefully with emphasis on a logical and user-friendly interface, and although the User Guide and Online Help contains modelling procedures and reference material, common sense is always needed in any practical application.

In this case, "common sense" means a background in ecological modelling, which is sufficient for you to be able to check whether the results are reasonable or not. Proper use of this Module requires knowledge about biological, and chemical processes in the water environment at a level of environmentally oriented engineers (civil engineer or chemical engineer) or model oriented biologists. A cooperation between engineers and biologists is recommended. It is assumed that you are familiar with the Hydrodynamic and Advection-Dispersion modules of MIKE 21. This Guide is not intended as a substitute for basic knowledge of the area in which you are working: environmental modelling of aquatic systems.

Advanced users might want to create their own MIKE ECO Lab templates. See the User Guide for MIKE ECO Lab templates in the manual called: MzGeneric.pdf.





# 2 Introduction

MIKE ECO Lab is a numerical lab for Ecological Modelling. It is an open and generic tool for customizing Aquatic Ecosystem models to describe water quality, eutrophication, heavy metals and ecology. The module is mostly used for modelling water quality as part of an Environmental Impact Assessment (EIA) of different human activities, but the tool is also applied in aquaculture for e.g optimization the production of fish, seagrasses and mussels. Another use is in online forecasts of water quality.

The need for tailormade ecosystem descriptions are big, because ecosystems vary. The strength of this tool is the easy modification and implementation of mathematical descriptions of ecosystems into the hydrodynamic engines of DHI.

The user can use Predefined MIKE ECO Lab Templates or can choose to develop own model concepts. The module can describe dissolved substances, particulate matter of dead or living material, living biological organisms and other components (all referred to as state variables in this context).

The module is developed to describe chemical, biological, ecological processes and interactions between state variables and also the physical process of sedimentation of components can be described. State variables included in MIKE ECO Lab can either be transported by advection-dispersion processes based on hydrodynamics, or have a more fixed nature (e.g. rooted vegetation).







# 3 Getting started

If MIKE ECO Lab is specified under Basic Parameters | Module Selection in a MIKE 21 Flow Model setup, then the ECO Lab dialogs will start.

In the Model Definition (Figure 3.1) dialog a MIKE ECO Lab template must be specified (.ecolab file). A MIKE ECO Lab template contains mathematical equations describing an aquatic ecosystem. The user has the option of using either:

1. one of the predefined DHI MIKE ECO Lab templates

or

other MIKE ECO Lab template. Choose 'From file...'

Having selected the MIKE ECO Lab template a brief summary of the contents is shown in the dialog.

Please note that every time a new template is selected, the specifications of all the remaining ECO Lab dialogs are reset to default values.

The specification of the Solution Parameters includes selection of the Integration Method for the coupled ordinary differential equations defined in the .ecolab file. At present the following three methods are available:

- Euler integration method
- Runge Kutta 4th order
- Runge Kutta 5th order with quality check

Finally the Update Frequency has to be specified. This parameter, which has to be an integer above zero, is defined such that:

#### $timestep(ECO\ Lab) = UpdateFrequency \times timestep(AD)$

The selection of the Time Step of the MIKE ECO Lab model, and hereby the Update Frequency, has to be based on considerations of the time scales of the processes involved. Please notice that this selection can be rather decisive for the precision of the numerical solution as well as for the CPU time of the simulation. A large Update Frequency will decrease the precision as well as the CPU time. It is therefore advisable to perform a sensitivity analysis on the Update Frequency before making the final selection.



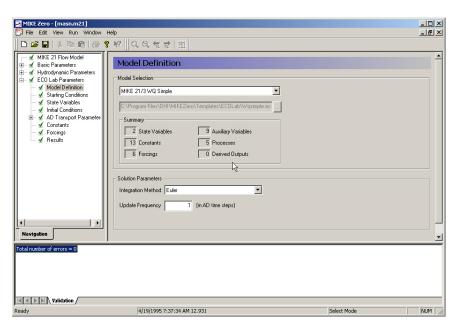


Figure 3.1 Dialog for choosing Model definition

In the Starting Conditions dialog (Figure 3.2) the user must choose between a socalled a 'Cold start' or a 'Hot start'.

If your simulation is to be a continuation of a previous one, then you must select the "Hot Start" option. The hot start facility requires a "hot file", i.e. a type 2 data file containing hot start data, for each model area. These must all have originated from the same simulation. The hot start files contain all necessary information to continue a simulation. In this way simulation time can be reduced if for instance a number of scenarios are to be simulated, all requiring identical starting conditions based on the same warm up period.

NOTE: You can let the MIKE ECO Lab part of the calculation be hot-started irrespective of the starting conditions of the Hydrodynamic part.



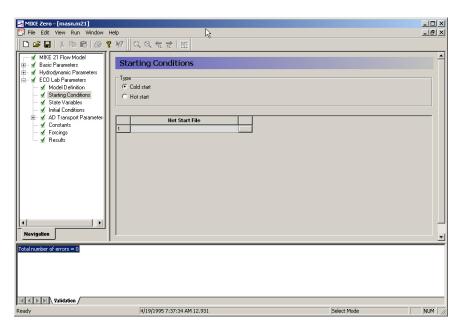


Figure 3.2 Dialog for choosing starting conditions

The State Variables Dialog (Figure 3.3) shows a summary of the State Variables defined in the MIKE ECO Lab model. The Symbol, Description, Unit and Transport type ("NONE" refers to a fixed State Variable and "AD" refers to a moveable state variable, which is transported by Advection-dispersion) of each State Variable are given.

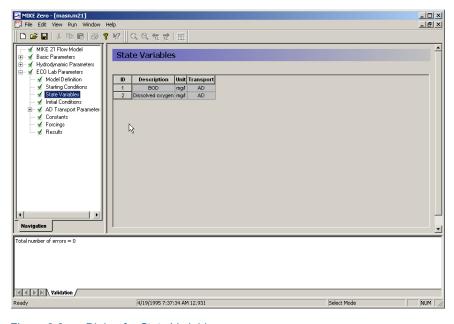


Figure 3.3 Dialog for State Variables



In the Initial Conditions dialog (Figure 3.3) initial concentrations for all state variables must be specified. For each State Variable you should specify its initial value within each computational area. You can specify the initial values in one of two ways:

- As a constant value applied to all points in the area; or
- From a type 2 data file with values given at each grid point.

For hot-started simulations, the initial values are read from the hot-data file(s).

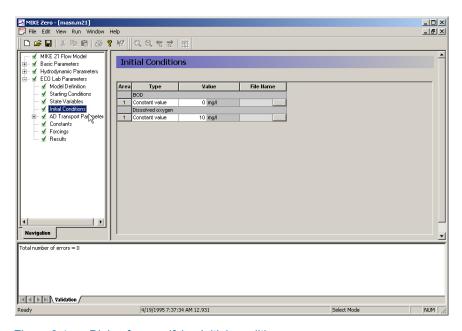


Figure 3.4 Dialog for specifying Initial conditions

In the Boundary dialog (Figure 3.5) boundary concentrations for all advective state variables must be specified at each open boundary in the model. The concentration at the open boundary can be specified in one of three ways:

- As a constant value, which will be used at all times at all grid points along the open boundary;
- From a type 0 data file with time-variant values, which will be used at all grid points along the open boundary; or
- From a type 1 data file where time-variant values are defined for each grid point along the open boundary

NOTE: At one open boundary you cannot mix the different types of boundary data. Also any possible data file (type 0 or 1) must have the same number of items as there are components in the simulation.



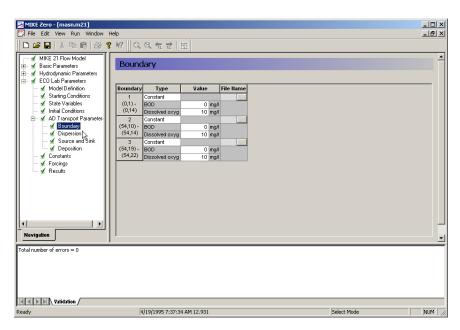


Figure 3.5 Dialog for specifying Boundary Concentrations

In the Dispersion dialog (Figure 3.6) Dispersion coefficients must be specified. On this dialog you specify the dispersion coefficients. The dispersion coefficients can be set either as independent of the current, or scaled in accordance with the calculated fluxes proportional to the current.

If you have selected "Independent of the current", you should specify the dispersion coefficients. You must specify a value for each spatial direction. For each area, you can specify the coefficients either as a constant value applied to all points in the area or as read from a type 2 data file.

If you have selected "Proportional to the current", you should specify a proportionality factor for each direction. With this selection, the dispersion coefficients are at all times scaled in accordance with the calculated fluxes. To avoid values that would make the computation unstable, reasonable cut-off limits should be specified.

NOTE: Remember that dispersion coefficients in a mathematical model are dependent on the grid size and time step, in addition to the physics of the problem.



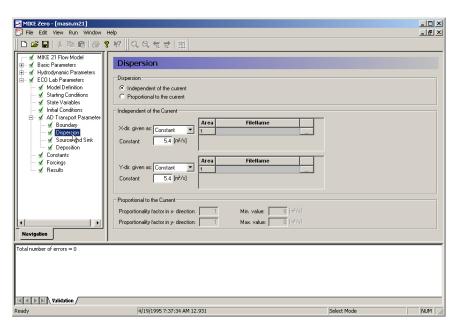


Figure 3.6 Dialog for specifying Dispersion Coefficients

In the Source and Sink dialog (Figure 3.7) Source and sink concentrations for all advective state variables must be specified.

For each State Variable, which are transported by Advection-dispersion, you should specify the concentration in each defined source in the model.

You can either specify the source concentration as constant in time or read and interpolate the concentration from a type 0 data file.

The total amount of mass discharged through a source is the concentration multiplied with the hydrodynamic discharge.

NOTE: At one source you cannot mix the two different types. Also, any possible data file must have the same number of items as the number of State Variables, which are transported by Advection-dispersion, in the simulation.



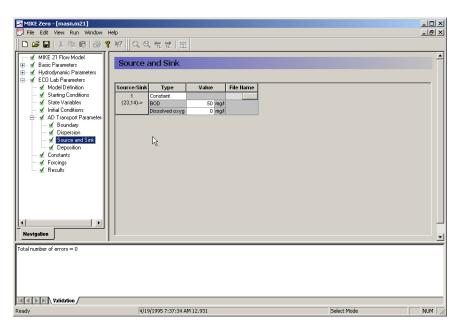


Figure 3.7 Dialog for specifying Source and Sink Concentrations

In the ECO Lab Constants dialog (Figure 3.8) the MIKE ECO Lab constants defined in the MIKE ECO Lab template can be modified.

The Constants are defined as any input parameter (physical constant, coefficient, rate, etc.) in the MIKE ECO Lab model, which is constant in time. The Constants are essentially divided into two groups:

- Built-in Constants; and
- User-specified Constants.

The built-in Constants are automatically provided by the model system during execution, whereas the user-specified Constants have to be specified in the present Dialog. Depending on the Spatial Variation of the Constant, as defined in the MIKE ECO Lab model, it can be specified as a "Constant value" or a "Type 2 data file" with one time step. In case a type 2 file is allowed for, a file for each model area has to be specified.

Please notice that a Constant, which is defined as a built-in Constant in the MIKE ECO Lab model, will appear as a user-defined Constant here in case it is not supported by MIKE 21 Flow Model.



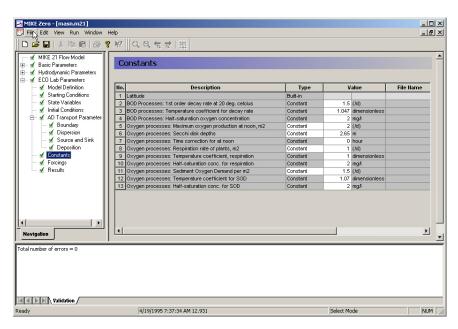


Figure 3.8 Dialog for specifying MIKE ECO Lab Constants

In the ECO Lab Forcings dialog (Figure 3.9) the MIKE ECO Lab forcings defined in the MIKE ECO Lab template can be modified. The Forcings are defined as any input parameter (physical property, rate, etc.) in the MIKE ECO Lab model, which is varying in time. Examples of a Forcing are: Temperature, salinity, solar radiation, and water depth. The Forcings are essentially divided into two groups:

- Built-in Forcings; and
- User-specified Forcings.

The built-in Forcings are automatically provided by the model system during execution, whereas the user-specified Forcings have to be specified in the present Dialog. Depending on the Spatial Variation of the Forcing, as defined in the MIKE ECO Lab model, it can be specified as a "Constant value", a "Type 0 data file" or a "Type 2 data file". The data files have to cover the entire simulation period. In case a type 2 file is allowed for, it must match the spatial extent of the main area.

Please notice that a Forcing, which is defined as a built-in Forcing in the MIKE ECO Lab model, will appear as a user-defined Forcing here in case it is not supported by MIKE 21 Flow Model.



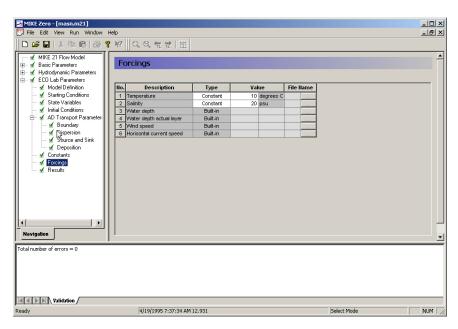


Figure 3.9 Dialog for specifying MIKE ECO Lab Forcings

The Mass Budget dialog (Figure 3.10) provides the user with a possibility to establish the mass budget of one or more State Variables within a certain area of the model domain. The specification of a mass budget comprises two steps: Firstly the area (or polygon) corresponding to the mass budget has to be defined and secondly the mass budget contents and output file have to be defined. The former is performed in the Basic Parameters Dialog whereas the latter is performed in the ECO Lab Parameters Dialog.

At first the number of mass budget files is specified. A mass budget file contains the mass budget of one or more State Variables. A mass budget of a State Variable consists of time series of:

- Total mass within polygon;
- Accumulated mass transported over lateral limits of polygon;
- Accumulated mass added/removed by external sources/sinks within polygon. (This item also includes any AD Solver mass corrections.);
- Accumulated mass added/removed by MIKE ECO Lab processes such as production or degradation within polygon; and
- Accumulated mass deviation (error) within polygon determined as the difference between the mass change and the transported, added and removed mass.

This means that for every Standard vs nested MIKE ECO Lab module selected, five items will be included in the corresponding mass budget file.



The mass budget file is thus defined by an associated polygon, information on which time steps to store, filename and title, and selected State Variables. Notice that the mass budget file is a Type 0 data file, since it contains simple time series.

The units of the masses in the mass budget file are defined as the equivalent of the unit of the corresponding State Variable multiplied by 106 m<sup>3</sup> for State Variables, which are transported by advection-dispersion, and 106 m<sup>2</sup> for fixed State Variables. This means that if the unit of the State Variable is [mg/l], the mass unit will be [metric tons]. Similarly the State Variable unit [g/m<sup>2</sup>] corresponds to a mass unit of [metric tons].

Notice that it is not possible to specify any mass budget files before one or more polygons have been specified under the Basic Parameters Dialog (see Mass Budget).

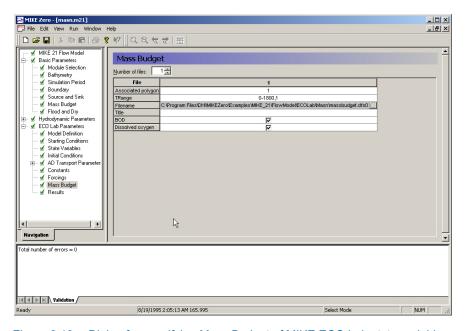


Figure 3.10 Dialog for specifying Mass Budget of MIKE ECO Lab state variables

In the Results dialog (Figure 3.11) the user can specify what output to save in a file.

You can specify the area and period of time from where the computed concentration fields should be written to a data file. All data types, type 0, 1, and 2 can be saved.

NOTE: These result files tend to be very big, so bear that in mind when selecting the area and period. In case of a Blow-up the last written Time Step might be corrupted, causing a read error when the file is processed from other tasks, e.g. plotting.



#### General description about results

Computers are not yet so powerful that a simulation can be run each time a plot of (say) the concentration field of one of the components is needed. Therefore it is necessary to store the basic results from the simulations. On the other hand, the amount of output produced by one single simulation is often so large that it is necessary to limit the amount of output saved.

#### Specifying the output area

On the Output Specifications menu you specify how many "output areas" (or output data files) you wish to have produced from the simulation. You can then specify the contents of each file:

- First, specify the associated model area of the output file.
- Specify the area to be included in the data file. By default the whole area
  is chosen but, if you are only interested in part of the model area, you
  could specify the area of interest only. The type of output data file(s)
  depends on the selected output area: If you specify a grid point a type 0
  data file will be generated, if you specify a grid line a type 1 data file will
  be generated, etc.
- Specify the range of time steps to be saved and whether every time step is to be included or only every second, third etc.
- Specify the output file name and location, and optionally a descriptive file title.
- Finally, select the State Variables, the additional output items and the velocity components to be included in the output file. Notice that the additional output items are defined by the MIKE ECO Lab model (the .ecolab file).

#### Remarks and hints

One way of following the progression of your simulation is by following the number of Time Steps written in the output data files (or one of them). In most post-processing tasks you start by specifying the data name after which you are presented with the description of the data. This description includes the number of time steps already written and thus finalised.



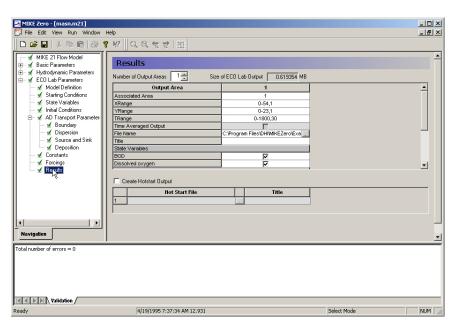


Figure 3.11 Dialog for specifying MIKE 21 Flow Model ECO Lab Results



# 4 Examples

#### 4.1 General

One of the best ways of learning how to use a modelling system such as MIKE 21 Flow Model ECO Lab Module is through practice. Therefore, an example has been included:

Masnedoe

The specification file for the example is included with the installation of MIKE Zero. The example can be found in the following directory:

.\Examples\MIKE 21\FlowModel\ECOLab\Masn

#### 4.2 Masnedoe

#### 4.2.1 List of data and specification files:

The following data files are supplied with MIKE 21:

Name: bathy.dfs2

Name: east.dfs0

Name: west.dfs0

Name: wind.dfs0

Specification file: masn.m21

# 4.2.2 Purpose of the example

The model illustrates a strait between two islands, and covers an area of 16 by 7 km. The model has one western boundary and two eastern boundaries. For the western boundary a flux varying with the tide has been applied, and for the eastern boundaries corresponding water level variations have been applied. An outfall, continuously discharging different oxygen demanding material, is simulated at point (23,14) with a discharge of 1.0 m3/s. The purpose is to determine BOD and dissolved oxygen concentrations caused by the single outlet. A concentration of dissolved oxygen of 10 mg/l will be used through the whole simulation at the open boundaries. The grid spacing is 300 meter and a time step of 240 seconds is used for the hydraulic as well as for the MIKE ECO Lab calculations.



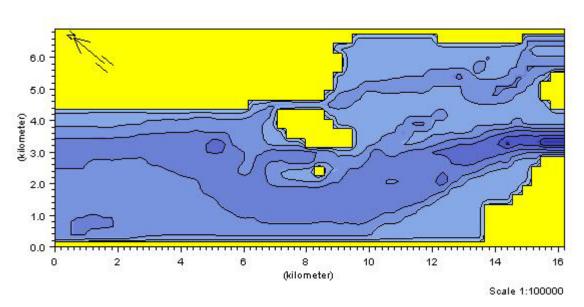


Figure 4.1 Bathymetry of Masnedoe example

### 4.2.3 Setting up the model

The hydrodynamic specifications will not be described since it is assumed that you are familiar with this part. After starting MIKE Zero you load this example by opening the file masn.m21.

The MIKE 21 Flow Model ECO Lab Module setup is divided into 7 ECO Lab dialogs plus additional dialogs related to advection-dispersion specifications for MIKE ECO Lab state variables.

- Model definition
- Starting conditions
- 3. State variables
- 4. Initial conditions
- Constants
- Forcings
- 7. Results

The advection-dispersion specifications for the MIKE ECO Lab Module are divided into 6 dialog types (they might not all be visible if no precipitation or evaporation are not specified in the hydrodynamic dialogs):

- 1. Boundary concentrations
- 2. Dispersion specifications



- 3. Source and sink
- Precipitation
- Evaporation
- 6. Deposition

In the **Modeldefinition** dialog the predefined template called M21/3 WQ Simple is picked. The integration method is also specified here as 'Euler'. The update frequency of the MIKE ECO Lab equations are specified. In this case the MIKE ECO Lab equations are updated with the same frequency as the hydrodynamic and the advection calculations.

Under **Starting conditions** a 'Cold start' is picked. This means that it will be necessary to specify initial conditions, see below.

The **State Variable** menu show which state variables that are included in the picked MIKE ECO Lab template: BOD and Dissolved oxygen (defined under Model definition). This menu is just used for getting information about state variables in the loaded MIKE ECO Lab template.

The **Initial Conditions** dialog specifies the initial conditions for BOD and Dissolved Oxygen:

BOD=0 mg/l

DO=10 mg/l

Under AD Transport Parameters:

Boundary concentrations should be specified

BOD=0

DO=10

Source concentrations should be specified under Source and Sink BOD=50

DO=0

- 3. Dispersion coefficients for the included state variables should be specified in the **Dispersion** dialog:
- 4. Deposition is not included in the example and nothing is therefore specified in the **Deposition** dialog.

In the example the dispersion coefficients are specified as 'independent of the currrent' with constant values:

X direction: 5.4 m2/s



Y direction: 5.4 m2/s

In the **Constants** dialog you should specify the constants that are defined in the template.See Table 4.1.

Table 4.1 Constant specification in the Masnedoe example

Constant description	Value
Latitude	Built-in (read in bathymetry)
BOD Processes. 1st order decay rate at 20 deg celcius	1.5 1/d
BOD Processes. Temperature Coefficient for decay rate:	1.047
BOD Processes. Halfsaturation oxygen concentration:	2.0 mg/l
Oxygen Processes. Maximum oxygen production at noon	2.0 g O2/m2/day EUM unit = 1/d
Oxygen Processes. Secchi Disk Depth	2.65 m
Oxygen Processes. Time correction for noon	0 hours
Oxygen Processes. Respiration rate of plants	1.0 g O2/m2/day EUM unit = 1/d
Oxygen Processes. Temperature Coefficient, respiration	1.0 (Dimensionless)
Oxygen Processes. Halfsaturation conc. for respiration	2.0 mg/l
Oxygen Processes. Sediment oxygen demand	1.5 g O2/m2/day EUM unit = 1/d
Oxygen Processes. Temperature coefficient for SOD	1.07 (Dimensionless)
Oxygen Processes. Halfsaturation conc. for SOD	2.0 mg/l



In the Forcings dialog you should specify the forcings that are defined in the

Table 4.2 Forcing specification in the Masnedoe example

Forcing description	Value				
Temperature	10 degrees C				
Salinity	20 psu				
Water depth	Built-in				
Water depth actual layer	Built-in				
Wind speed	Built-in				
Horisontal current speed	Built-in				

MIKE ECO Lab template. See Table 4.2.

In the **Results** dialog you should specify the output that you wish to see.

After simulation you can extract timeseries of the results. In Figure 4.2 and Figure 4.3 simulated timeseries of BOD and DO concentrations are shown for a point near the source and a point 1300 meters away from the source. After the first couple of days the concentrations have become stationary and the concentration variations of BOD and DO follow the tidal flow. It can be seen that both the dissolved oxygen and BOD concentrations are affected by the source.

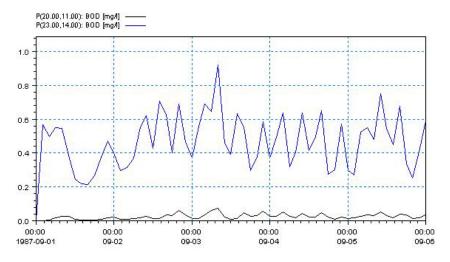


Figure 4.2 Concentrations of simulated BOD (mg/l) at the source point and 1300 m form the source



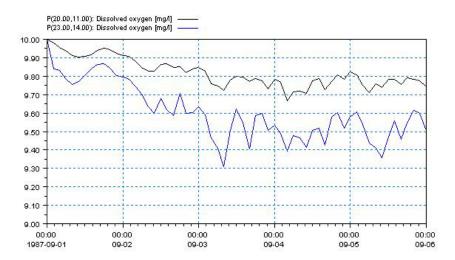


Figure 4.3 Concentrations of Dissolved Oxygen (mg/l) at the source point and 1300 m from the source



## 5 Reference Manual

It is intended that you use this manual when you are doing model applications of MIKE ECO Lab and need to know how various inputs, output etc. can be specified. Also often used terms in MIKE ECO Lab are explained.

All the entries listed below are included in the Reference Manual in alphabetic order.

Additional output items

**Auxiliary Variable** 

Blow-up

**Boundary Conditions** 

**Built-in Constants** 

**Built-in Forcings** 

**Built-in Functions** 

Calibration

Constant

Courant Number

**CPU Time** 

**Deposition Concentration** 

**Derived Output** 

Disk Space

**Dispersion Coefficients** 

Euler integration method

Eutrophication MIKE ECO Lab template

**Evaporation Concentrations** 

Expression

Forcing

Heavy Metal MIKE ECO Lab template

Hot Data

Infiltration Concentrations

**Initial Concentrations** 

Mass Budget

Mathematical functions

**Output Area** 

**Precipitation Concentrations** 

Predefined MIKE ECO Lab Templates

**Processes** 

**Process Matrix** 

Process Type

References

Reserved words

Runge Kutta 4th order

Runge Kutta 5th order with quality check

Sources and Sinks

Semantic Rules

**Spatial Variation** 



Standard vs nested MIKE ECO Lab module Syntax rules of expressions Temperature dependencies Time Step Transport Units Water Quality MIKE ECO Lab templates

# 5.1 Additional output items

When specifying results in MIKE ECO Lab applications it is possible to choose state variables and additional output. The list of additional output is specified in the MIKE ECO Lab template and can be:

- 1. Auxiliary variables
- Processes
- Derived output

# 5.2 Auxiliary Variable

Auxiliary variables are mostly arguments in mathematical expressions of Processes in a MIKE ECO Lab template, but sometimes they are only used for specifying results directly.

They are defined as mathematical expressions themselves with a sequence of arguments and operators.

Arguments in a auxiliary variable expression could be state variables, constants, forcings, numbers, or other auxiliary variables. The auxiliary variables are calculated in the order they are defined in the MIKE ECO Lab model, starting from top. So only auxiliary variables defined above the present auxiliary variable expression can be used as argument in auxiliary variable expressions.

The idea is to split long process expressions (see processes) into subexpressions under auxiliary variables, so that the process expressions become more simple and easier to read. However, only the model developers imagination limits the possible use of auxiliary variables, because here you can calculate intermediate results. Typical examples of auxiliary variables are dimensionless factors that can be multiplied a process. The factors could for instance be a factor for primary productions dependency of light, or a factor for coliform bacterias decay dependency of temperature. The defined factor is then used as argument under processes. Other uses of auxiliary variables are to use them in other auxiliary variables. For instance an auxiliary variable for estimating light in the water column can be used as argument in the auxiliary variable mentioned above for calculating a factor for primary productions dependency of light.



# 5.3 Blow-up

Please inspect carefully the description in the **log** file.

# 5.4 Boundary Conditions

#### 5.4.1 General description

Just as with the hydrodynamic set-up, the concentrations at the open boundaries are of great importance for advection-dispersion calculations. In the situation where the flow is out of the open boundary, the concentrations at the boundary for all advective state variables are calculated automatically. When the flow is running into the model the concentrations must be specified at the boundary.

Because you very seldom are able to tell beforehand whether the flow is running out of the model, concentrations have to be specified at all time steps. When the flow is directed out of the model, the internally calculated values are used instead of the specified boundary values.

You can specify the boundary concentrations in one of the following ways:

A constant value used throughout the whole simulation. The value is applied at all points along the boundary.

A time series (type 0 data file) which automatically is interpolated to match the simulation time step. Again the value at a time step is applied at all points along the boundary. The data file must have the same number of items, as there are components in the simulation. This means, that if you want to use a type 0 data file for your boundary concentrations, the values for all the components have to be in that file.

A time series of line values (type 1 data file) which automatically is interpolated to match the simulation time step. The number of grid points in the data file must match the number of grid points along the open boundary. In addition the data file must have the same number of items, as there are components in the simulation. This means, that if you want to use a type 1 data file for your boundary concentrations, the values for all the components have to be in that file.

The file can be generated by the type 1 data editor (the Profile Editor) or by the advection-dispersion transfer data program in the "Environment" section of the MIKE 21 Toolbox.

For all the different ways of specifying boundary values, it is necessary to specify them for all open boundaries and for all components.



**NOTE** that the number and the position of open boundaries are given via input under the Boundary (p. 24) section under Basic Parameters Dialog Overview (p. 19).

#### 5.4.2 Hint

Normally you should, if possible, place the open boundaries away from both the areas of interest and areas of influence. Doing this, the boundary concentrations can be given as the background concentration.

#### 5.5 Built-in Constants

It is possible in MIKE ECO Lab templates to refer to constants that are specified or calculated in the hydrodynamic engines of MIKE. The available built-in constants are not the same in all the hydrodynamic engines. If it is specified that it should be a built-in constant and it is not available in the engine, the engine dialog will prompt as if the constant was user specified.

It is possible to choose from the following list of built-in constants:

- Latitude. If available this built-in constant returns the latitude of the model area.
- Longitude. If available this built-in constant returns the longitude of the model area.
- Bed level. If available this built-in constant returns the altitude of the model area.
- AD time step (AD\_DT). This built-in constant returns the time step in seconds between every advection-dispersion calculation.
- ECO Lab time step (WQ\_DT). This built-in constant returns the time step in seconds between every update by the MIKE ECO Lab module

# 5.6 Built-in Forcings

It is possible in MIKE ECO Lab templates to refer to forcings that are specified or calculated in the hydrodynamic engines of MIKE. The available built-in forcings are not the same in all the DHI hydrodynamical engines. If it is specified that it should be a built-in forcing and it is not available in the engine, the engine dialog will prompt as if the forcing was user specified.

It is possible to choose from the following list of built-in forcings:



- Water layer height. This forcing returns the spatial distance between layers (in meters). In one layered grid systems the water depth will be returned
- Salinity. If available this forcing returns the salinity calculated in the hydrodynamic setup
- Temperature. If available this forcing returns the temperature calculated in the hydrodynamic setup
- Wind velocity. If available this forcing returns the wind velocity specified in the hydrodynamic setup
- 5. Wind direction. If available this forcing returns the wind direction specified in the hydrodynamic setup
- Water surface level. This forcing returns the water level calculated in the hydrodynamic setup
- Water depth. This forcing returns the water depth calculated in the hydrodynamic setup
- 8. Horizontal current speed. This forcing returns the horizontal current speed in meters per second calculated in the hydrodynamic setup
- 9. Horizontal current direction. This forcing returns the horizontal current direction in degrees calculated in the hydrodynamic setup
- Vertical current speed. This forcing returns the vertical current speed in meters per second calculated in the hydrodynamic setup
- 11. Water surface slope in flow direction. This forcing returns the slope of the water surface (meter per meter) calculated in the hydrodynamic setup. Under normal conditions positive values.
- 12. Bed area of grid cell
- 13. Flooded area of grid cell
- Surface area of grid cell
- 15. Volume of grid cell
- 16. Horizontal grid cell flux
- 17. Vertical grid cell flux
- 18. Water density. If available in hydrodynamic simulation this forcing returns a value for water density

## 5.7 Built-in Functions

It is possible in MIKE ECO Lab templates to choose from a database a number of predefined functions and use them in the expressions. The database contains the following functions:



- Daynumber(Year, Month, Day). This function returns an integer between 1 and 365 representing the daynumber in year.
- Arrhenius20(TemperatureCoefficient,Temperature). This function returns a temperature dependency based on the following Arrhenius expression:

$$f(a,b) = a^{(b-20)}$$
 (5.1)

3. Arrhenius5(TemperatureCoefficient,Temperature). This function returns a temperature dependency based on the following Arrhenius expression:

$$f(a,b) = a^{(b-5)}$$
 (5.2)

4. Oxygensaturation(Salinity,Temperature). This function returns an estimate of the saturated dissolved oxygen concentration in the water as function of salinity and temperature:

$$f(a,b) = \begin{pmatrix} 14,65-0,0841 \cdot a + b(0,00256 \cdot a - 0,41022 + b \\ (0,007991-0,0000374 \cdot a - 0,000077774 \cdot b)) \end{pmatrix}$$
(5.3)

 OxygensaturationWeiss(Salinity,Temperature). This function returns an estimate of the saturated dissolved oxygen concentration in water as function of salinity and temperature. Suggested by Weiss.

 Lassiter(LassiterConstant,GrowthRate,GrowthOptimumTemperature, GrowthInhibitionTemperature,Temperature). This function returns a dimensionless temperature dependency factor relevant for many biological processes.

Lassiter(a, b, c, d, temp) = 
$$b \cdot e^{a(temp-c)} \cdot \frac{d-temp}{d-c}^{a \cdot (d-c)}$$
 (5.5)

7. MichaelisMenten1(Concentration, HalfsaturationConstant):

$$f(a,b) = \frac{a}{a+b} \tag{5.6}$$



MichaelisMenten2(Concentration, Constant):

$$f(a,b) = \frac{a^2}{a^2 + b} ag{5.7}$$

ReverseMichaelisMenten(Concentration):

$$f(a) = \frac{1}{a+1} \tag{5.8}$$

- 10. Sunrise (Year, Month, Day, Latitude, Correction For Summer Time)
- 11. Sunset (Year, Month, Day, Latitude, Correction For Summer Time)
- LambertBeer1(SurfaceLight,LayerHeight,LightExtinctionCoefficient).
   This function estimates the light penetration in water column based on Lambert Beer expression. The lightintensity in the top of each gridlayer is returned.
- LambertBeer2(SurfaceLight,LayerHeight,LightExtinctionCoefficient)This
  function estimates the light penetration in water column based on Lambert Beer expression. The lightintensity in the bottom of each gridlayer is
  returned.
- RelativeDaylength(Month,Day,Latitude). Returns a value for relative daylength. The value equals 1 at equinox (when day and night have same length).

#### 5.8 Calibration

By calibration of a MIKE ECO Lab setup in MIKE 11/21/3 ECO Lab) it is attempted to find the best accordance between computed and observed state variables (model components) by variation of a number of parameters.

Deviation between computed and observed state variables in MIKE ECO Lab can be caused by a number of reasons. The most obvious are:

- 1. Inaccurate specification of concentrations at the model boundaries
- 2. Inaccurate specification of loadings to the ecosystem
- Inaccurate initial concentrations
- 4. Inaccurate hydrodynamic setup
- 5. Limitations in the chosen MIKE ECO Lab process descriptions
- Inaccurate calibration of coefficients in MIKE ECO Lab process equations
- 7. Wrong measurements
- Instable numerical solution



The MIKE ECO Lab modeller should when calibrating a MIKE ECO Lab setup have the above mentioned possible reasons for inaccuracy in the results in mind, before changing parameters dramatically.

Calibrating coupled ordinary differential equations can be tricky, because of the mutual dependency of the state variables. So if one state variable is calibrated to fit the observed values, maybe it will not fit so well after calibrating other state variables in the ecosystem. Some dependencies are stronger than others. Therefore it is advisable to calibrate the state variables with the least dependencies to other state variables first.

For the DHI MIKE ECO Lab templates the following calibration order is suggested:

## 5.8.1 EU Eutrophication template:

Recommended calibration order

Phytoplankton

Potential growth, shift diatoms-green algae

Sedimentation

Light extinction

Temperature dependency

- Nutrients
- Detritus sedimentation/decay
- Sediment (denitrification/immobilisation)
- Oxygen
- Macrophytes

## 5.8.2 WQ Water Quality Templates:

Recommended calibration order

BOD-DO relations

degradation rates

re-aeration

production/respiration

(nitrification)

Nutrients



content BOD

nitrification/denitrification

sorption processes

Coliforms

#### 5.9 Constant

Constants are used as arguments in the mathematical expressions of processes in a MIKE ECO Lab template. They are constant in time, but can vary in space. Typical examples of constants are different specific rate coefficients, exponents, halfsaturation concentrations and also universal constants such as gas constant and atomic weights.

Hint: Some coefficients and transformation rates can be found in the litterature, but many have not been documented in litterature. So this possible lack of information is wise to investigate, before defining a complex MIKE ECO Lab model.

#### 5.10 Courant Number

#### 5.10.1 General description

The transport Courant number in the x-direction is defined as follows:

$$C_{rx} = U \cdot \frac{\Delta t}{\Delta x} \tag{5.9}$$

where U is the current speed,  $\Delta t$  the time step and  $\Delta x$  the grid spacing.

The Courant number actually expresses how many grid points the information or the given matter moves in one time step.

#### 5.10.2 Recommended value

The final Courant number is calculated as the sum of the Courant number in the x-direction and the Courant number in the y-direction. The sum of these two must be below 1.0. See further under Time Step (p. 60).



#### 5.11 CPU Time

#### 5.11.1 Factors influencing the CPU time

The CPU time required by a hydrodynamic and MIKE ECO Lab simulation depends on the size of your model, on the number of time steps in your simulation, on the complexity of the used MIKE ECO Lab template, on the chosen numerical solution method and on the general computational speed of your computer.

If you wish to estimate how a change in your model specifications for the hydrodynamic part changes the CPU time required without specifying the model setup and doing a verification, please refer to your HD Reference Manual (p. 71).

However, if you wish to estimate how changes in your MIKE ECO Lab set-up changes the CPU time required, the following guidelines can be used:

- the CPU time varies linearly with the number of water points (or computational points) in the model.
- the CPU time also varies linearly with the number of time steps.
- the CPU time increases approximately linearly with the number of advective state variables.

# 5.12 Deposition Concentration

# 5.12.1 General Description

Deposition of state variable concentrations is implemented as so-called dry deposition. Dry deposition is as a source term in the advection-dispersion calculation without a corresponding HD term. We distinguish between two different types of dry deposition

- Surface Deposition (p. 40), e.g. pollution from air.
- Soil Deposition (p. 41), e.g. leaching from highly contaminated sea bed.

# 5.12.2 Surface Deposition

You may choose to include surface deposition in your AD simulation. If you do so, you must also specify how the component concentrations should change due to deposition through the water surface.

You may specify the deposition rate (in units of the state variables unit times cubic metres per second) as "Constant value", "Type 0 data file" or "Type 2 data file".



# 5.12.3 Soil Deposition

You may choose to include soil deposition in your AD simulation. If you do so, you must also specify how the component concentrations should change due to deposition from the seabed.

You may specify the deposition rate (in units of component's unit times cubic metres per second) as "Constant value", "Type 0 data file" or "Type 2 data file".

# 5.13 Derived Output

Derived output is additional output that the user can specify in MIKE ECO Lab templates. They are usually results that are not given in the state variables directly, but as can be derived from the state variables or processes.

Derived output are described as mathematical expressions with a sequence of arguments and operators. Arguments in a derived output expression could be state variables, constants, forcings, auxiliary variables, numbers, or processes. It is not possible to refer to derived output in other expressions.

Examples of derived output in a MIKE ECO Lab model could be Total N or Secchi depth that both are not given directly through the state variables, but can be derived from them. It shall be noted that the derived output is calculated after the state variables have been integrated, so identical expressions including state variables as arguments, will not give the same result if calculated under auxiliary variables instead of under derived output.

# 5.14 Disk Space

#### 5.14.1 Small files

The disk space required for your simulation depends mainly on the amount of results you request to be saved. During a simulation only two or three other files, in addition to the data files containing the results are created:

- the specification file containing the simulation specifications. This file will
  be placed in your present working directory and have a file extension of
  m21. It will only take up approximately 6 Kbytes.
- the log file describing the model setup, the statistics of the files used and created during the simulation and a message for each time step completed. The file extension of this file, which will also be placed in your present working directory, is log and it will take up to 300 Kbytes on the disk.



 a file for the continuation of a simulation, the hot file. This file only takes up disk space equivalent to 'the number of components' times the space taken up by the bathymetry file. This mean that the hot file will not take up more space than 100 - 200 Kbytes (depending on your setup).

## 5.14.2 Large files

The amount of data generated by a simulation is very large. Therefore you should only save as much data as is needed for your further work. Nevertheless very large files will often be generated.

#### 5.14.3 Remarks and hints

Please note that MIKE 21 does not check whether or not you have enough free disk space for your requested output files.

# 5.15 Dispersion Coefficients

#### 5.15.1 General description

Physical flow processes occur simultaneously at different spatial and temporal scales with a continuous spectrum ranging from molecular agitation to tidal, barotropic and baroclinic residual flows. The need to express conservation laws by means of mathematical methods imposes the treatment of fluid motions as part of continuum mechanics. This implies the use of spatial scales much larger than the intermolecular spacings associated with molecular agitation processes, in order to define the properties such as concentrations. Furthermore, for the study of practical problems only the flow processes above a certain minimum scale are of interest, hence the direct modelling of smaller scales giving rise to unnecessary and in practice unaffordable computational costs. By using convenient filtering procedures it is possible to avoid the explicit inclusion of those scales in the dependent variables used in the mathematical formulations. These non-resolved scales can not be ignored, as part of the energy of the flow is absorbed by them. Therefore they have to be empirically related to the dependent variables (that are representative of all the resolved scales) through specific terms that naturally appear as a consequence of the filtering procedures. The relationships to be used and the respective empirical coefficients will then reflect the existence of non-resolved scales, the main effects of which can be classified as follows:

Dissipative, which account for the amount of energy present in the non-resolved scales or/and the decay/growth of flow properties. In two-dimensional hydrodynamic models for example, bottom friction explains not only the energy losses due to shear stresses, but also the total amount of energy contained in the non-resolved scales along the vertical.



 Dispersive, which account for the transfer of energy or properties between resolved scales, due to the existence of non-resolved scales. These effects are represented by the so-called viscosity/diffusion coefficients.

The wide range of time and length scales involved, as well as the variability of flow conditions, makes it impossible to develop a unified approach with universally applicable expressions for the evaluation of the referred empirical coefficients. Therefore one has to resort to calibration values through the use of reliable and sufficient data. However the values of those coefficients are subject to large variations, thus raising the need for good first estimates, that can be obtained both by theoretical analysis of the physical processes and through the use of experience acquired in similar applications.

# 5.15.2 Specifying the dispersion coefficients

Dispersion coefficients are required, whenever there are moving state variables.

The dispersion coefficients can be:

- specified as constant in space, as a coefficient for the x-direction and a coefficient for the y-direction.
- specified as two-dimensional maps of coefficients, similar to the bathymetry map or a resistance map.
- calculated every time step, proportional to the hydrodynamic current densities. If you choose this formulation, proportionality constants, minimum and maximum values are also required.

#### 5.15.3 Recommended selection and values

Selecting dispersion coefficients is very difficult. The optimum method is to obtain the coefficients from a calibration process, where simulated and measured concentration fields are compared. Very seldom are measurements available for calibration of transport processes. These processes have very long response times (months or years), and therefore, empirical estimates have to be utilised.

Many different formulations can be applied e.g.

D = 
$$K_1 \Delta x^2 / \Delta t$$
,  
D =  $K_2 \Delta x u$   
or  
D =  $K_3 \Delta t u^2$ 



∆x is the grid spacing, ∆t is the time step and u is the local current speed.

#### 5.15.4 Remarks and hints

Using too high values of the dispersion coefficients, will cause instabilities. The stability is a function of the local transport courant number and the dispersion coefficient. For practical applications it is not possible prior to a simulation, to judge whether the upper limit of the dispersion coefficients have been reached. If you insist on using a specific value of the dispersion coefficient, even though you get instabilities, you must decrease the time step.

When running the MIKE 21 Flow Model, Advection-Dispersion Module the program does not accept all values, since an upper limit can be reached:

$$\left(\frac{D_x}{\Delta x^2} + \frac{D_y}{\Delta y^2}\right) \cdot \Delta t < 0.5 \tag{5.10}$$

This is based on the stability criteria for a pure diffusive problem, where the upper limit is 0.5.

# 5.16 Euler integration method

A very simple numerical solution method for solving ordinary differential equations.

The formula for the Euler method is:

$$y_{n+1} = y_n + hf(x_n, y_n)$$

which advances a solution y from  $x_n$  to  $x_{n+1} = x_n + h$ 

# 5.17 Eutrophication MIKE ECO Lab template

Predefined DHI supported MIKE ECO Lab template that is a model of eutrophication processes in aquatic systems.

See scientific description of the EU template under manuals in the installation. The pdf file can be viewed directly from the MIKE ECO Lab template editor when the EU template is loaded.



# 5.18 Evaporation Concentrations

When evaporation occurs or when the net-precipitation is negative, you need to specify how the component concentrations should change due to evaporation. There are two different ways to do this:

- You may choose the format "Ambient water" concentration, in which
  case the concentration of the evaporated water mass is set equal to the
  concentration of the ambient sea water.
- You may specify the value of the the concentration in the evaporated water mass through the formats "Constant value", "Type 0 data file" or "Type 2 data file".

If you have chosen the net-precipitation option, then the selected format for "Evaporation concentrations" will be used when the specified net-precipitation is negative. When the net-precipitation is positive, an precipitation concentration as specified under Precipitation Concentrations (p. 49) is applied.

# 5.19 Expression

Expressions must be specified for state variables, auxiliary variables, processes, and derived output in the MIKE ECO Lab templates. An expression is a sequence of arguments and operators.

The expressions must follow the Syntax rules of expressions and the Semantic Rules.

# 5.20 Forcing

Forcings are used as arguments in the mathematical expressions of processes in a MIKE ECO Lab template. They can vary in time and space. They represent variables of an external nature that affect the ecosystem. Typical examples of forcings are temperature, solar radiation and wind.

Hint: If many measurements are available of a state variable, it is possible to temporarily replace it with a forcing. This way a specific process can be isolated and calibrated with less uncertainty. After calibrating the process, the forcing can be transformed back into a state variable again.

# 5.21 Heavy Metal MIKE ECO Lab template

Predefined DHI supported MIKE ECO Lab template that is a model for estimating the spreading of heavy metals in aquatic systems.

See scientific description of the ME template under manuals in the installation. The pdf file can be viewed directly from the MIKE ECO Lab GUI when the ME template is loaded.



#### 5.22 Hot Data

## 5.22.1 General description

You can start your simulation either from scratch (a "cold start") or on the basis of a previous simulation (a "hot start"). In the latter case you need to save information about the simulation you wish to continue. These data are called "hot data".

The MIKE ECO Lab hot data file contains the following model information:

 Initial conditions for state variables based on last time step in previous simulation.

Thus, if you use a hot start, you need not (and cannot) specify the data listed above.

## 5.22.2 Specifying the hot data

You specify that you wish to be able to continue the MIKE ECO Lab simulation by first enabling the "Generate Hot Start" on the Results (HD) dialog, and then writing the **name** of the HD hot data file.

Then you specify that you wish to be able to continue the simulation you are about to execute by enabling the "Generate Hot Start" on the Results (MIKE ECO Lab) dialog, and then writing the **name** of the MIKE ECO Lab hot data file.

You specify that you wish to do a simulation as a continuation of a previous one by selecting "hot Start" on the Starting Conditions (MIKE ECO Lab) dialog, and then writing the **name** of the hot data file created earlier.

# 5.23 Infiltration Concentrations

If you have included infiltration in your simulation you need to specify how the concentration of the State Variables, which are transported by Advection-dispersion, shall change due to infiltration. There are two different ways to do this:

 You may choose the format "From Ambient Water", in which case the concentration of the infiltrated water mass is set equal to the concentration of the ambient sea water.



 You may specify the value of the concentration in the infiltrated water mass through the formats "Constant value", "Type 0 data file" or "Type 2 data file".

The constant value will be applied to all points in the model, at all time steps. The type 0 and type 2 data file must cover the whole simulation period and have the same number of items as there are State Variables, which are transported by Advection-dispersion, in the simulation. The type 2 data file must match the spatial extent of the main area.

#### 5.24 Initial Concentrations

A specification of the starting concentrations is required for all the MIKE ECO Lab state variables in a simulation. There are two possibilities: A **Constant Value** used everywhere in the model or the starting concentrations can be **Read from Type 2 Data File.** 

# 5.25 Mass Budget

The mass budget facility provides the user with a possibility to establish the mass budget of one or more state variables within a certain area of the model domain. The specification of a mass budget comprises two steps: Firstly the area (or polygon) corresponding to the mass budget has to be defined and secondly the mass budget contents and output file have to be defined. The former is performed in the Basic Parameters Dialog whereas the latter is performed in the MIKE ECO Lab Parameters Dialog.

At first the number of mass budget files is specified. A mass budget file contains the mass budget of one or more MIKE ECO Lab state variables. A mass budget of a state variable consists of time series of:

- Mass within polygon
- Accumulated mass transported over lateral limits of polygon
- Accumulated mass added/removed by sources/sinks within polygon.
- Accumulated mass added/removed by "internal" processes such as decay within polygon
- Accumulated mass deviation (error) within polygon determined as the difference between the mass change and the transported, added and removed mass

This means that for every state variable selected, five items will be included in the corresponding mass budget file.

The mass budget file is thus defined by an associated polygon, information on which time steps to store, filename and title, and selected model components. Notice that the mass budget file is a Type 0 data file, since it contains simple time series.



The units of the masses in the mass budget file are defined as the equivalent of the unit of the corresponding model component multiplied by 10<sup>6</sup> m<sup>3</sup>. This means that if the unit of the model component is mg/l, the mass unit will be 10<sup>9</sup> mg, i.e. metric tons.

Notice that it is not possible to specify any mass budget files before one or more polygons have been specified under the Basic Parameters Dialog Mass Budget.

#### 5.26 Mathematical functions

It is possible to use a number of mathematical functions in expressions in the MIKE ECO Lab templates. Here is a list of the supported mathematical functions:

The syntax below must be followed carefully with respect to capital letters and number of arguments.

- 1. ABS(X)
- 2. ARCCOS(X)
- 3. ARCSIN(X)
- ARCTAN(X)
- 5. ARCTAN2(X,Y)
- 6. COS(X)
- 7. COSH(X)
- 8. EXP(X)
- 9. LN(X)
- 10. LOG(X)
- 11. MAX(X,Y)
- 12. MIN(X,Y)
- 13. POW(X,Y)
- 14. SIN(X)
- 15. SINH(X)
- 16. SQR(X)
- 17. SQRT(X)
- 18. TAN(X)
- 19. TANH(X)
- 20. PI()



# 5.27 Output Area

## 5.27.1 General description

Computers are not so powerful that a simulation can be run each time a plot of, for example, the concentration field is needed. Therefore it is necessary to store the basic results from the simulations. On the other hand, the amount of output produced by a single simulation is often so large that it is necessary to limit the amount of output saved.

## 5.27.2 Specifying the output area

On the Results (MIKE ECO Lab) dialog you specify how many output data files you wish to have produced from the simulation. You can then specify the contents of each data file:

- you specify the data name and data title,
- you specify the area to be included in the data file. By default the whole
  area is chosen but, if you are only interested in a part of the model area
  and you have finished the calibration, you could specify the area of interest only.
- you specify the range of time steps to be saved and if every time step should be included or only every second, third or whatever.
- you specify the output items to save from a list

#### 5.27.3 Remarks and hints

One way of following the progress of your simulation is to follow the number of time steps written in your output file (or one of them). In most postprocessing tasks you start by specifying the data file name and after having done so, you are presented with the description of the data. This description includes the number of time steps already written and thus finished.

# 5.28 Precipitation Concentrations

If your simulation includes precipitation, you need to specify how the advective state variable concentrations should change due to precipitation. There are two different ways to do this:

You may choose the format "Ambient water" concentration, in which
case the concentration of the precipitated water mass is set equal to the
concentration of the ambient sea water.



 You may specify the value of the the concentration in the precipitated water mass through the formats "Constant value", "Type 0 data file" or "Type 2 data file".

If you have chosen the net-precipitation option, then the selected format for "Precipitation concentrations" will be used when the specified net-precipitation is positive. When the net-precipitation is negative, an evaporation concentration as specified under Evaporation Concentrations (p. 45) is applied.

# 5.29 Predefined MIKE ECO Lab Templates

DHI has a number of standard MIKE ECO Lab templates.

EU.ecolab: Eutrophication
 ME.ecolab: Heavy metal

3. COLI.ecolab: Coliform bacteria

4. WQSimple.ecolab: BOD-DO

5. WQNutrients.ecolab: BOD-DO, nutrients

6. WQlevel1.ecolab: BOD-DO (especially for MIKE 11!!)

7. WQsimpleCOLI.ecolab: BOD-DO and Coliform bacteria

8. WQsimpleTandS.ecolab: BOD-DO and temperature and salinity

9. WQsimpleTandSCOLI.ecolab: BOD-DO, Coliform bacteria and temperature and salinity

#### 5.30 Processes

Processes are arguments in differential equations governing the state of the state variables included in MIKE ECO Lab templates.

They are defined as mathematical expressions themselves with a sequence of arguments and operators. Arguments in a process expression could be state variables, constants, forcings, auxiliary variables, numbers, or other processes. The processes are calculated in the order they are defined in the MIKE ECO Lab model, starting from top. So only processes defined above the present process expression can be used as argument in process expressions. Examples of processes in a MIKE ECO Lab model could be degradation, death, or production of a state variable. All processes can be described as rates i.e. they relate to time.

# 5.31 Process Matrix

A process matrix show the interaction between state variables and processes. It is a simple way of getting an overview of a MIKE ECO Lab models state variables and which processes affect them. All defined processes are



listed in rows and all state variables are listed in columns. Any interaction between a state variable and a process is included by specifying a coefficient at the appropriate place in the process matrix. A positive coefficient should be specified if the process increases the state of the state variable, and a negative value if the influence of a process decreases the value of a state variable. The process matrix of a template can be seen in the MIKE ECO Lab template editor by choosing 'Tools: Processmatrix'.

# 5.32 Process Type

The model developer has the following process types to choose from when defining a process in a MIKE ECO Lab template:

- Transformation. This is for instance in situ degradation, production, of matter. This process type transformates matter at the spot, and can not move or transport matter
- Settling. This process moves matter down the water column, and in mulitlayered gridsystems the matter is moved from layer to layer.

#### 5.33 References

A tool for viewing dependencies of a symbol to other symbols. The references of a symbol can be seen in the MIKE ECO Lab template editor by choosing 'Tools: references' when a symbol is marked.

### 5.34 Reserved words

MIKE ECO Lab has reserved the following list of words for special functionality in the expressions of an MIKE ECO Lab template. So they can only be used in expressions for that functionality.

- 1. YEAR, returns present year in simulation
- MONTH returns present month in simulation
- 3. DAY returns present day in simulation
- 4. HOUR returns present hour in simulation
- MINUTE returns present minute in simulation
- SECOND returns present second in simulation
- PI() returns the value for pi: 3.14.....
- 8. Logical functions
- Mathematical functions



# 5.35 Runge Kutta 4th order

A classical numerical solution method for solving ordinary differential equations. It has usually higher accuracy than the Euler method, but requires longer simulation times. The fourth order Runge-Kutta method requires four evaluations of the right hand side per time step.

$$k_1 = hf(x_n, y_n) ag{5.11}$$

$$k_2 = hf\left(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right)$$
 (5.12)

$$k_3 = hf\left(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}\right)$$
 (5.13)

$$k_4 = hf(x_n + h, y_n + k_3)$$
 (5.14)

$$y_{n+1} = y_n + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} - O(h^5)$$
 (5.15)

# 5.36 Runge Kutta 5th order with quality check

A numerical solution method for solving ordinary differential equations. The accuracy is evaluated and the time step is adjusted if results are not accurate enough.

It requires 6 function evaluations for each time step to take a socalled Cash-Karp Runge Kutta step and the error is estimated as the difference between a Runge Kutta fourth order solution and the Runge Kutta fifth order solution.

# 5.37 Scope

Scope is the MIKE ECO Lab way of specifying in the MIKE ECO Lab template where a state variable or process can be found in the water environment. By having this description of the physical distribution of state variables and their processes it is possible to control that the state variables are only affected by a process in locations, where the state variables and the processes have overlapping occurrence.

A process or state variable with scope WS (water surface) has the physical meaning that it is located in the upper part of the water column and it is always in direct contact with the water surface. Note that a WS State variable not touches the water bed. An example of a WS state variable can for



instance be water hyacinths. An example of a WS process could be reaeration (exchange of oxygen between water phase and atmosphere). A WS process or state variable is only represented by one number per horizontal gridpoint.

A process or state variable with scope WC (water column) has the physical meaning that it can be located in the whole water column. This means that a WC state variable can both touch the water surface, the water bed, or neither. An example of a WC state variable can for instance be phytoplankton Carbon concentration. An example of a WC process that akes place in the whole water column could be BOD degradation. If a state variable is specified as WC and it is affected by a WS process, the process will only influence the state variable in the water surface layer. In all other layers the process will be set to zero. A WC process or state variable is represented by one number per vertical layer per horizontal gridpoint.

A process or state variable with scope WB (water bed) has the physical meaning that it is located in the bottom part of the water column and it is always in contact with the bed. Note that a WB state variable can not touch the water surface, but dependent on the discretization of the water column in a specific model setup a situation where both state variables that are confined to the bed and to the water surface can exist in the same model point. This is always the case for depth integrated model systems. Examples of a WB state variable can for instance be eelgrass, macroalgae, or filtrators. An example of a WB process could be release of inorganic nitrogen from the sediment. A WB process or state variable is only represented by one number per horizontal gridpoint.

A process or state variable with scope SED (sediment) has the physical meaning that it is located in the sediment. Only transformation processes are possible in the sediment and processes defined as WS processes (for instance oxygen exchange with atmosphere) can not influence a SED state variable. SED state variables have a fixed nature and can not be transported by the advection dispersion module of the hydrodynamic engines. An example of a SED state variable can for instance be BOD in the sediment.

A SED process or state variable is only represented by one number per horizontal gridpoint. Therefore if the modeller wants the sediment to be divided into layers, each layer should be defined as separate SED state variables. Example: State variable 1: ammonia in porewater (layer 1), State variable 2: ammonia in porewater (layer 2) etc.

# 5.38 Semantic Rules

The semantic rules define how arguments in expressions of a MIKE ECO Lab template can be combined by excluding combinations that from a logical point of view make no sense. The rules are about



- which spatial variation combinations that can be combined
- 2. which scopes of processes and state variables that can be combined.

The rules are as follows:

#### 5.38.1 State variables

Spatial variation is not user specified for State Variables. Instead state variables assumed to always have spatial variation 'HORISONTAL\_AND\_VERTICAL'. This cannot be changed by the user. 'Scope' is specified for the state variables. Legal arguments to an expression for a differential equation specified under state variables are only numbers and Processes. The following arguments are legal in state variable expressions:

- Processes with spatial variation 'NONE', 'HORISONTAL' or 'HORISONTAL\_AND\_VERTICAL'. All scopes of the processes are legal. If for instance scope of a process is chosen as WS and used in a state variable expression. The process will have a value when calculating the top layer of the water column, but the process will have the value zero in other layers.
- 2. Numbers.

## 5.38.2 Auxiliary variables

Scope is not user specified for Auxiliary Variables, but spatial variation must be specified and the options are 'NONE', 'HORISONTAL', and 'HORISONTAL\_AND\_VERTICAL'.

Legal arguments to an expression for an auxiliary variable with spatial variation 'NONE' are:

 already defined auxiliary variables, constants, forcings with spatial variation 'NONE'

Legal arguments to an expression for an auxiliary variable with spatial variation 'HORISONTAL' are:

- already defined auxiliary variables, constants, forcings with spatial variation 'NONE' or 'HORISONTAL'
- state variables with scope 'WS', 'SED', or 'WB'

Legal arguments to an expression for an auxiliary variable with spatial variation 'HORISONTAL\_AND\_VERTICAL' are:



- already defined auxiliary variables, constants, forcings with spatial variation 'NONE' or 'HORISONTAL' or 'HORISONTAL\_AND\_VERTICAL'
- 2. state variables with scope 'WS', 'SED', 'WB', or 'WC'

#### 5.38.3 Processes

Both spatial variation and scope must be specified for processes.

Legal arguments to an expression for a process with spatial variation 'NONE' are:

1. already defined processes, auxiliary variables, constants, forcings with spatial variation 'NONE' and all scope types are legal.

Legal arguments to an expression for a process with spatial variation 'HORI-SONTAL' are:

- already defined processes, auxiliary variables, constants, forcings with spatial variation 'NONE' or 'HORISONTAL'
- already defined processes with spatial variation 'HORISON-TAL\_AND\_VERTICAL' with scope 'WS', 'SED', or 'WB'
- state variables with scope 'WS', 'SED', or 'WB'

Legal arguments to an expression for a process with spatial variation 'HORI-SONTAL\_AND\_VERTICAL' are:

 already defined state variables, processes, auxiliary variables, constants, and forcings. Conflicts between scope or spatial variation for the arguments are not possible here.

#### 5.38.4 Derived output

Scope is not user specified for Derived Output, but spatial variation must be specified and the options are 'NONE', 'HORISONTAL', and 'HORISONTAL AND VERTICAL'.

Legal arguments to an expression for a Derived Output with spatial variation 'NONE' are:



1. processes, auxiliary variables, constants, forcings with spatial variation 'NONE'

Legal arguments to an expression for a Derived Output with spatial variation 'HORISONTAL' are:

- processes, auxiliary variables, constants, forcings with spatial variation 'NONE' or 'HORISONTAL'
- 2. state variables with scope 'WS', 'SED', or 'WB'

Legal arguments to an expression for a Derived Output with spatial variation 'HORISONTAL AND VERTICAL' are:

- processes, auxiliary variables, constants, forcings with spatial variation 'NONE' or 'HORISONTAL' or 'HORISONTAL AND VERTICAL'
- 2. state variables with scope 'WS', 'SED', 'WB', or 'WC'

#### 5.39 Sources and Sinks

#### 5.39.1 General description

The effects of rivers, intakes and outlets from power stations etc. can be included in a simulation. These sources and sinks are included in both the hydrodynamic and the advection-dispersion calculation. The source/sink positions and discharges are specified in the Basic Parameters Dialog Overview (p. 19) and HD Dialog Overview (p. 29) part, respectively, whereas the source concentrations are specified in the MIKE ECO Lab parameters dialog.

There are three different ways of specifying sources and sinks:

1:Isolated Source.

Here you specify the source concentration, constant or varying in time for each component.

2:Isolated Sink.

Isolated sinks are only processed in the hydrodynamic part.

3:Source - Sink Pair.

Here it is possible to deal with 'connected sources', several sources connected to one sink (or 'connected sinks'), several sinks connected to one source. This is done in the way that the concentration at the sink point is added to the user defined source(s) concentra-



tion. In the hydrodynamic part you ensure that the sum of the connected source discharges are the same as the sink discharges.

This Source-Sink Pair feature is normally used in cooling water investigations for power plants. For example, the 'heated water source' is connected to a number of sinks in the power plant area. By using a Source-Sink Pair it is possible to investigate the recirculation of heated water; is it likely that the water temperature in the environment increases continuously?

You can specify the source concentrations of the advective state variables in one of the following ways:

- A constant value used throughout the whole simulation.
- A time series (type 0 data file) which automatically is interpolated to
  match the simulation time step. The date file must have the same number of items, as there are components in the simulation. This means that
  if you want to use a type 0 data file for your source concentration, the values for all the components have to be in that file.

# 5.40 Spatial Variation

For constants, forcings, auxiliary variables, processes, and derived output the model developer has to specify in the MIKE ECO Lab template editor what variation pattern that can be expected for the variable. The options are:

- None
- 2. Horizontal
- Horizontal and vertical

When specifying spatial variation for auxiliary variables, processes, and derived output, that all contain expressions, the model developer should be careful that the spatial variation of the variable is not conflicting with the specified spatial variations of the used arguments in the expression. See Semantic Rules.

## 5.41 Standard vs nested MIKE ECO Lab module

# 5.41.1 General Description

The purpose of this section is to enable the user to use the Nested MIKE ECO Lab module of the MIKE 21 Flow Model. As most features in nested MIKE ECO Lab are identical to the features in the standard MIKE ECO Lab, this manual only describes the nested facilities.



The nested MIKE ECO Lab module in MIKE 21 Flow Model, solves the MIKE ECO Lab equations simultaneously with advection-dispersions calculations in a user defined number of dynamically nested grids, and runs coupled with the nested hydrodynamic module.

The advantage of applying the nested grid facility compared to the standard of using only one grid is mainly the reduced CPU time requirements. Typical applications of the MIKE ECO Lab modules have a limited physical area of main interest, which is only a smaller part of the total modelling area. To obtain a satisfactory spatial resolution of the model within this area of interest, the standard advection-dispersion module can be used, but will often result in a very large number of computational grid points (and often within areas of only limited interest for the application), and accordingly will require much CPU time. Applying the nested module, the spatial resolution can be optimised to save computer time.

## 5.41.2 Nested Model Specifications

As the nested MIKE ECO Lab module runs coupled with the MIKE 21 FLow Model, Nested Hydrodynamic Module, the rules laid out in *Standard vs. nested HD module (p. 98)*, should be followed.

Most MIKE ECO Lab model specifications are identical in standard MIKE ECO Lab and Nested MIKE ECO Lab, but a few comments regarding the differences are listed below:

- Initial concentration for state variables should be specified for each area.
- Dispersion coefficients, which are specified as constants, are common for all model areas.
- Dispersion coefficients, which are specified as two-dimensional maps should be specified for each model area.
- Dispersion coefficients, which are proportional to the current, are common for all model areas.
- Constants with spatial variation 'NONE' in MIKE ECO Lab are common for all areas, whereas constants with spatial variation must be specified for each model area.
- As in MIKE 21 NHD, sources and sinks are specified in the model area
  of the finest resolution, which covers the actual geographical position of
  the source/sink.
- In the output specifications, each output area must be related to an associated model area.
- Hot input/output files must be specified for each model area.



#### Time step

The time step to be used in a Nested MIKE ECO Lab simulation is determined in the same way as in standard MIKE ECO Lab (based on the maximum transport Courant number). In the nested version though, it is necessary to calculate the transport Courant number within each model area based on the grid spacing, the current speed and the time step (which is the same in all grids) and then base the time step on the maximum of these transport Courant numbers. (Remember also to check the dispersion stability criteria for each model area, cf Dispersion Coefficients (p. 42)).

## 5.42 State Variable

State variables are usually the most important variables in a MIKE ECO Lab template. State variables represent those variables that describe the state of the ecosystem and that the user wants to predict the state of. So they are also the main result after running a MIKE ECO Lab setup. The state variable will change according to the processes that the model developer describes affect it. So the critical task for the model developer is to describe the processes in a way, so that the state of the state variable changes correctly, also when forcings (external conditions such as e.g. wind, temperature) change.

# 5.43 Syntax rules of expressions

Expressions in MIKE ECO Lab can be written in 2 ways:

- 1. Logical function: IF (expression) THEN (expression) ELSE (expression)
- 2. Normal expression: Expression

Expressions are sequences of arguments separated by operators.

List of legal arguments in expressions:

- Symbols for state variables, constants, forcings, auxiliary variables, processes defined in the MIKE ECO Lab model above the present expression
- 2. Built-in Functions from MIKE ECO Lab database, see built-in functions
- 3. Mathematical functions written in capital letters, see mathematical functions
- 4. Reserved words written in capital letters, see reserved words
- Numbers

The legal operators are multiplication, division, subtraction, addition.

See also Semantic Rules.



# 5.44 Temperature dependencies

## 5.44.1 General description

A large number of reactions in the environment are temperature dependent. Reactions involving biological elements are directly affected due to increased biological activity at higher temperatures. If the temperature rises above the optimum temperature for the biological reaction, the process rate will decrease. Chemical reactions can also increase with increasing temperature partly owing to the higher molecular activity.

## 5.44.2 Arrhenius temperature dependency factor

An often used simple expression for describing the temperature dependency of a process. It is described by a reference temperature (in most cases 20 deg Celcius) and a temperature coefficient:

The expression is available in the database of MIKE ECO Lab in a pre-compiled version. See also Built-in Functions.

Hint: It shall be noted that this expression grows exponentially with temperature, so for biological processes it shall only be used for temperatures below the optimum temperature.

# 5.44.3 Lassiter Temperature dependency factor

An often used expression for describing the temperature dependency of a biological process. The expression is available in the database of MIKE ECO Lab in a pre-compiled version. See also Built-in Functions.

# 5.45 Time Step

# 5.45.1 Selecting the time step

The time step for the advection-dispersion update of MIKE ECO Lab is the same as the one used for the hydrodynamic simulation, but the update of the MIKE ECO Lab equations can be chosen to be updated less frequent than the hydrodynamic and the advection-dispersion update. Therefore both the hydrodynamic model, the advection-dispersion model must be considered when selecting the hydrodynamic time step. Separately the MIKE ECO Lab model must be considered, when selecting the MIKE ECO Lab time step.

The procedure for selecting the hydrodynamic and the advection-dispersion time step is:



- first you determine the grid spacing, -x, as described under Bathymetry (p. 49),
- then you decide on the maximum allowed Courant number, C<sub>r</sub>, as described under Courant Number (p. 70),
- then you can determine the maximum time step,  $\Delta t_{max}$ , which can be used in the model from the definition of the Courant number:

$$\Delta t_{max} = \Delta x \cdot \frac{C_r}{c} \tag{5.16}$$

where c is the wave celerity (see Courant Number (p. 70) for a description). The time step to be used in the hydrodynamic model,  $\Delta t$ , can then be chosen as a "convenient" number not greater than  $\Delta t_{\text{max}}$ .

 finally you have to check that the Courant number based on the current speed, (the transport courant number) C<sub>r,tr</sub>, instead of the wave celerity, is less than 1 for the time step chosen. If not, you must reduce the chosen time step. C<sub>r,tr</sub> is defined as

$$C_{r,tr} = \Delta t \cdot \left(\frac{U}{\Delta x} + \frac{V}{\Delta y}\right) \tag{5.17}$$

where U,V is the current speed in the x-direction and y-direction. For all points within the model U and V must follow the above formula. As you have not yet carried out the simulation you will have to make an estimate and then check this after the simulation.

**Please note**, that formally U and V in the above expression should be replaced by P/H and Q/H, respectively, where P and Q are the magnitudes of the fluxes in the x- and y- directions and H is the local water depth. Often the two expressions – based on current speeds or on the flux magnitudes – yield almost the same value, but care should be taken in models with large surface and/or bottom gradients.

Then the time step for updating the MIKE ECO Lab equations must be selected relative to the chosen hydrodynamic time step. It is possible to choose the same time step or a longer time step than the hydrodynamic time step (multiple of the hydrodynamic time step). Many environmental processes changes less dramatic than hydrodynamics and advection-dispersion processes, and therefore it is often adequate to update MIKE ECO Lab much less frequent than the hydrodynamics. For instance a MIKE ECO Lab time step of a ½ hour for the DHI supported template 'EU.ecolab' is often used, which is rarely seen in hydrodynamic time steps.

The purpose of not updating the MIKE ECO Lab every time step is to reduce simulation time.



# 5.46 Transport

In MIKE ECO Lab the state variables that are present in the water column has the option of using the advection-dispersion module for calculating the transport based on hydrodynamics. If this option is not specified in the MIKE ECO Lab Template the state variable will have a fixed location and the calculation of its state will only be based on the processes defined in MIKE ECO Lab template and not based on advection-dispersion processes.

State variables that are present in the sediment can not be transported based on the advection-dispersion module.

It is also possible to have state variables in the water column that have a fixed nature. An example of that could be relevant in models involving aquaculture, for instance cages of scallops in the water column.

#### 5.47 Units

In MIKE ECO Lab it is possible to use a limited number predefined unit types that are supporting the EUM unit conversion system.

For state variables there are 3 unit types to choose from in the MIKE ECO Lab template editor.

- Volume Concentration [mg/l]. In the engine dialogs of MIKE ECO Lab
  this unit can be converted to other units for mass and volume chosen by
  the user.
- Area Concentration [g/m2]. In the engine dialogs of MIKE ECO Lab this
  unit can be converted to other units for mass and area chosen by the
  user.
- Undefined, here some user specified text can be written that will be written in e.g. output, but no conversion will take place by the EUM unit conversion system.

For processes the unit is always relating to time, so formally the unit is [per second], but it should be understood as [undefined per second]. This way the user has the option of changing the time unit to for instance [per hour] in the engine dialogs of MIKE ECO Lab, while the 'undefined' part of the unit will not be converted according to the EUM system.

For constants, forcings, auxiliary variables the units are not supported by the EUM unit conversion system, but it is possible to specify user specified text, that will be written in e.g. output and dialogs.



# 5.48 Water Quality MIKE ECO Lab templates

Predefined DHI supported MIKE ECO Lab templates that are a series of simple water quality models.

State variables that are modelled with the WQ templates are:

- 1. BOD
- 2. DO
- 3. Nitrate
- Nitrite
- 5. Phosphate
- Faecal Coliform
- Total Coliform

See scientific description of the WQ template collection under manuals in the installation. The pdf file can be viewed directly from the MIKE ECO Lab GUI when a WQ template is loaded.





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