MIKE 3 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 3 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 3 Flow Model 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 3. 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. How to do this is explained in the MIKE ECO Lab User Guide.

2 Introduction

MIKE ECO Lab is a numerical lab for Ecological Modelling. It is an open and generic tool for customising 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 optimisation the production of fish, seagrasses and mussels. Another use is in online forecasts of water quality.

The need for tailor made 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 3 Flow Model setup, then the MIKE 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

2. 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 MIKE 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 MIKE ECO Lab template. The following three integration method are available:

1. Euler integration
2. Runge Kutta 4th order
3. 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:

$$timestep(ECOLab) = UpdateFrequency \times timestep(AD)$$

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.
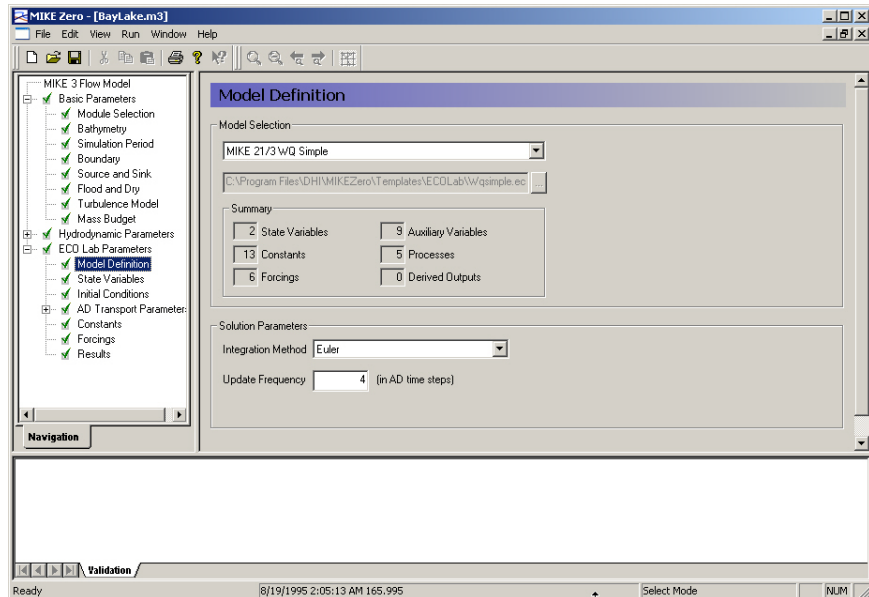
Figure 3.1   Dialog for choosing Model definition

A hot start means a continuation of a previous simulation. Initial conditions for state variables will be copied from a socalled 'Hot file' generated in a previous simulation. If a cold start is picked then the user must specify initial concentrations for all state variables. The hotfile can be specified in the dialog under Basic Parameters | Bathymetry.

The State Variable dialog (figure 3.2) gives a short description of the state variables included in the chosen MIKE ECO Lab template.
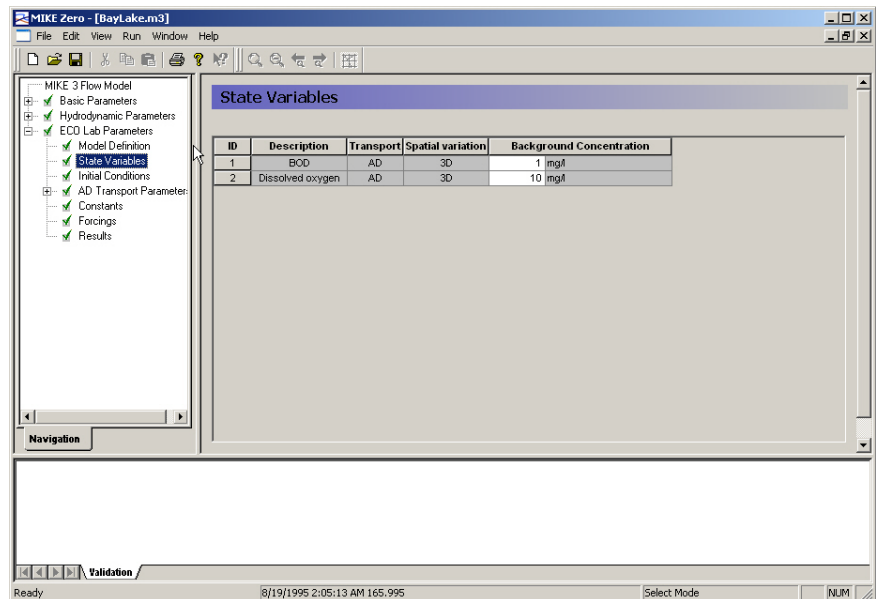
Figure 3.2   Dialog for State Variables

In the Initial Conditions dialog (figure 3.3) initial concentrations for all state variables must be specified. You must specify initial values 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/type 3 data file with values given at each grid point. Whether a type 2 or a type 3 data has to be specified depends on the spatial variation of the State Variable.

For hot-started simulations, the initial values are read from the hot-data file(s), which are specified in the Basic Parameters section.
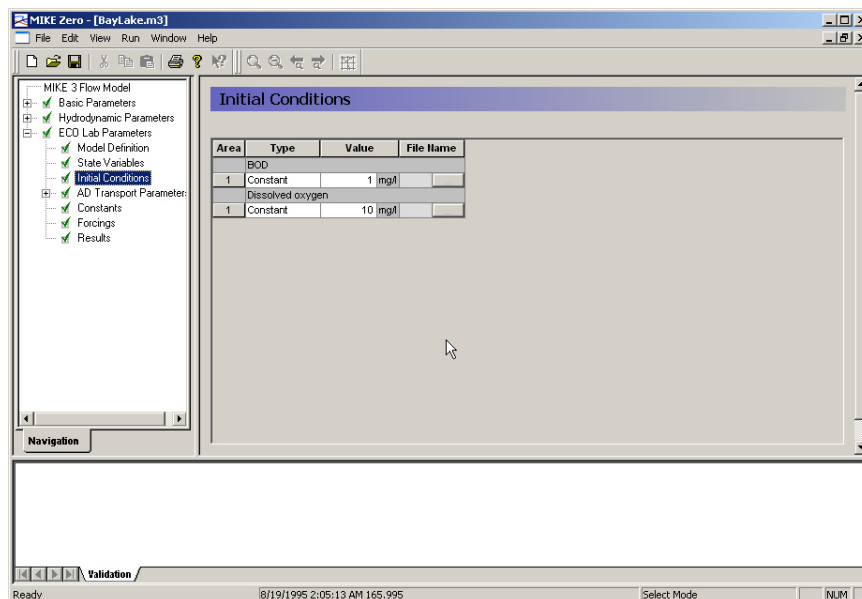
Figure 3.3   Dialog for specifying Initial conditions

In the Boundary dialog (figure 3.4) boundary concentrations must be specified.

At each open boundary in the model you should specify the concentration of each of the State Variables, which are transported by Advection-dispersion.

The concentration at the open boundary can be specified in four ways:

- As a constant value;

- As a time series (type 0 data file), the instantaneous value of which will be used at all grid points along the open boundary;

- From a type 1 data file where each horizontal grid point along the open boundary is defined; or

- From a type 2 data file where all grid point along the open boundary are defined.
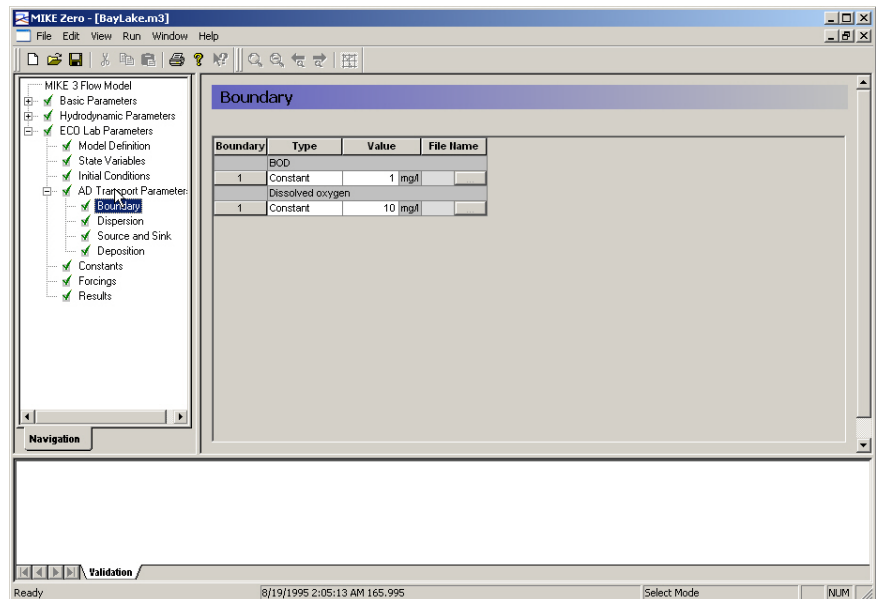
Figure 3.4   Dialog for specifying Boundary Concentrations

In the Dispersion dialog (figure 3.5) dispersion coefficients must be specified.

On this menu you specify the dispersion of each State Variable, which is transported by Advection-dispersion. You should specify the dispersion proportionality factors and set limits on the dispersion coefficients in all three directions. You may select the dispersion to be proportional to the local Eddy Viscosity, the local velocity or the local current speed (tensor dispersion).

A linear relationship is assumed between the dispersion of the components and the eddy viscosity, the velocity or the current speed, respectively. Dispersion factors define this linear relationship. To control dispersion the various parameters can be set differently for different model areas.

To control the dispersion, a lower and upper dispersion limit in each direction must be specified. Hereby you can avoid unreasonable dispersion coefficients, which could make the computation unstable. If you want to use a constant dispersion coefficient, simply set the maximum value equal to the minimum value.

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

See Reference Manual for details about specifying dispersions coefficients.
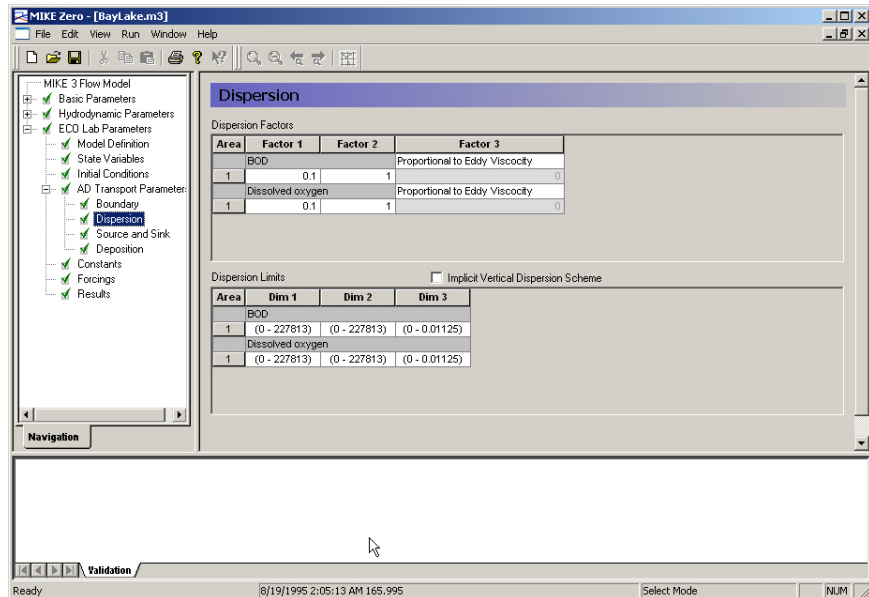
Figure 3.5   Dialog for specifying Dispersion Coefficients

In the Source and Sink dialog (figure 3.6) Source and sink concentrations must be specified.

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

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

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.

Notice that for sinks (negative discharge), the specified concentration is not made use of, and, for connected source-sinks, the specified concentration represents the excess concentration.

The total amount of mass discharged through a source is the concentration multiplied with the hydrodynamic discharge.
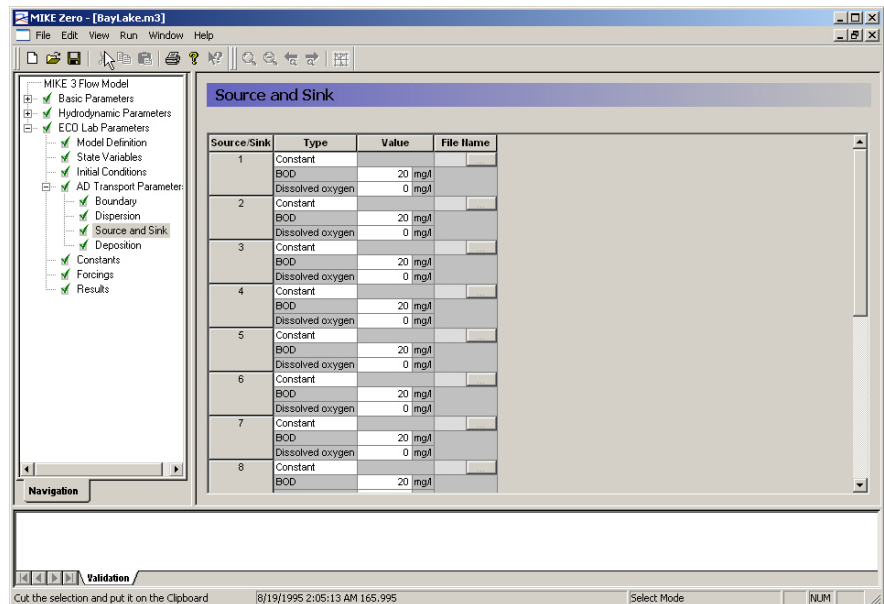
Figure 3.6   Dialog for specifying Source and Sink Concentrations

In the MIKE 3 ECO Lab Constants dialog (figure 3.7) the constants defined in the MIKE ECO Lab template can be changed. The Constants are defined as any input parameter (physical constant, numerical 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

● The 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" or a "Type 2 File" with one time step. In case a type 2 data file is allowed for, a file for each model area can be specified.
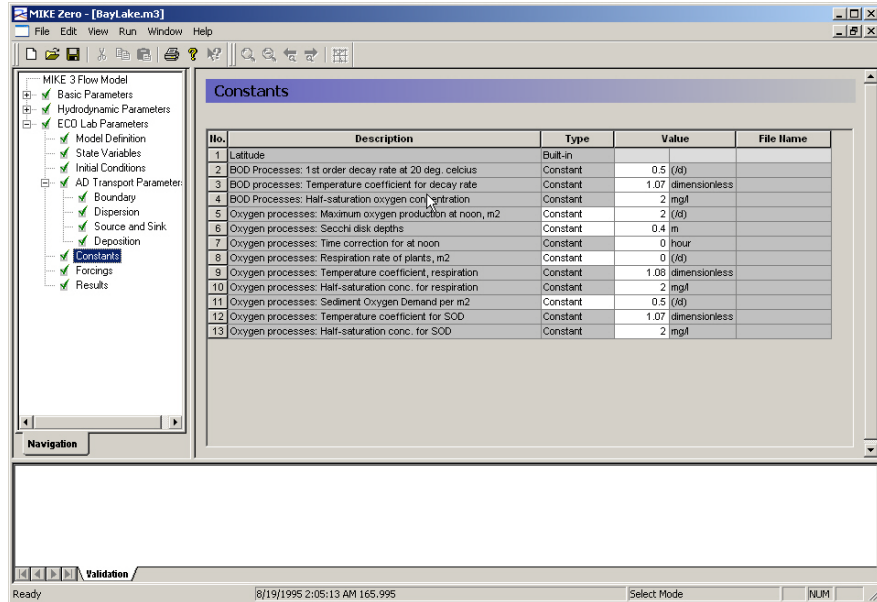
Figure 3.7   Dialog for specifying MIKE ECO Lab Constants

In the MIKE ECO Lab Forcings dialog (figure 3.8) the forcings defined in the MIKE ECO Lab template can be changed. The Forcings are defined as any input parameter (physical property, numerical property, rate, etc.) in the MIKE ECO Lab model, which is varying in time. Examples of a Forcing are: Temperature, solar radiation, water depth, and water layer height. The Forcings are essentially divided into two groups:

- The Built-in Forcings; and
- The 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", as a "Type 0 File" or as a "Type 2 File". The data files have to cover the entire simulation period. In case a type 2 data file is allowed for, it must match the spatial extent of the main area.
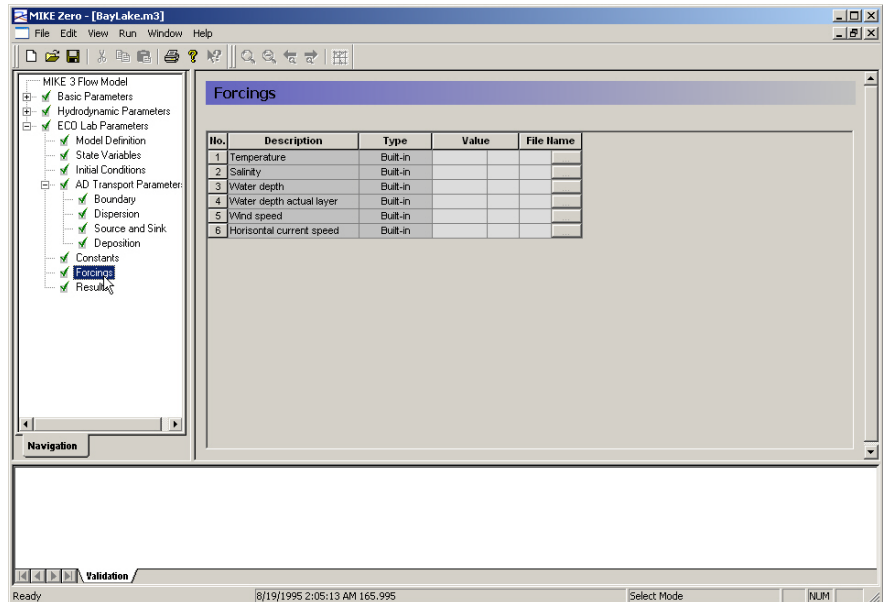
Figure 3.8   Dialog for specifying MIKE ECO Lab Forcings

In the Mass Budget dialog (figure 3.9) the user can specify mass budget files to include in setup.

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 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 includes precipitation, dry deposition and 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, file name 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^3 for State Variables, which are transported by advection-dispersion, and 106 m^2 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^2] 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 in Reference Manual).
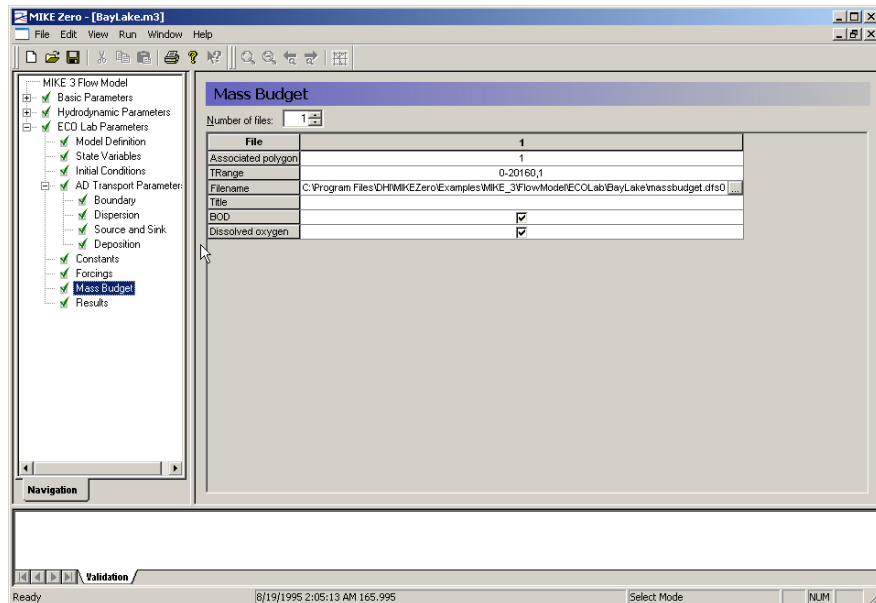
Figure 3.9   Dialog for specifying MIKE 21 ECO Lab massbudget

In the Results dialog (figure 3.10) the user can specify what output to save in a file.

On the Results menu 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:

• 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, and the Derived Output items and the velocity components to be included in the output data file. Notice that the additional output items are defined by the MIKE ECO Lab model (the .ecolab file). Notice also that items, which have a spatial variation of horizontal, cannot be included in an output data file with vertical (z-direction) variation.
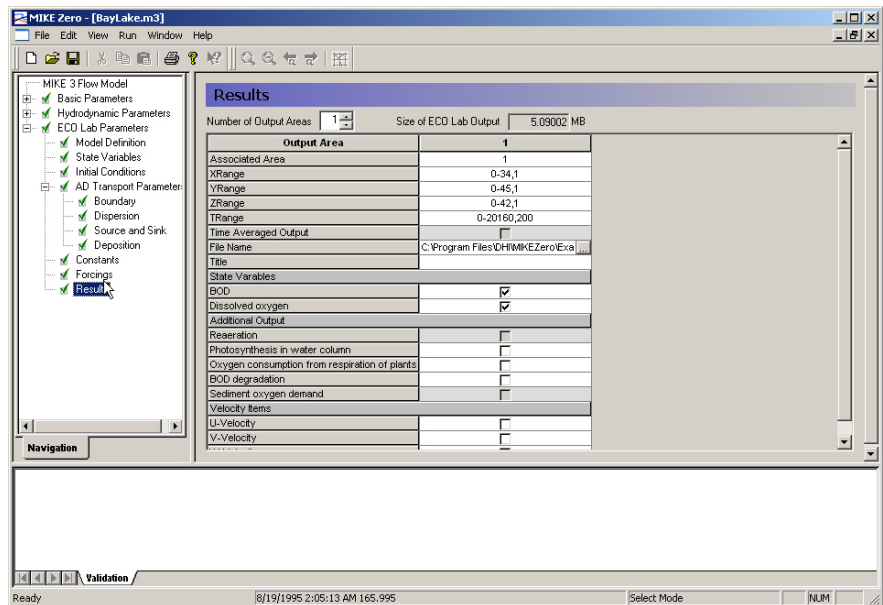
Figure 3.10   Dialog for specifying MIKE ECO Lab Results

4　Reference Manual

It is intended that you use this manual when you are making model applications of MIKE ECO Lab and need to know how various inputs, outputs, 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
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
Source and Sink
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

4.1 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

2. Processes

3. Derived output

4.2 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 bacteria's 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.

4.3 Blow-up

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

4.4 Boundary Conditions

4.4.1 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.

- 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 horizontal grid points along the open boundary, i.e. the boundary concentration will be vertically constant. The file may be generated by several means, e.g.: using the type 1 data editor (**ProfileEditor**), using the MIKE 21 advection-dispersion transfer data program with results from a previous MIKE 21 AD run, or using the tools in the MIKE Zero Toolbox to extract line series from 2D and 3D data.

- A time series of values at a vertical section (type 2 data file) which automatically is interpolated to match the simulation time step. The number of grid points, both horizontally and vertically, in the data file must match the number of grid points at the open boundary. There are several ways to generate such a file of boundary values, e.g.: You may use the type 2 data editor (**GridEditor**) or the tool in the MIKE Zero Toolbox to extract 2D data from a type 3 data file.

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 in the Boundary dialog in the Basic Parameters Dialog Overview section in the User Guide for the Hydrodynamic Module.

4.4.2 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.

4.5 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:

1. Latitude. If available this built-in constant returns the latitude of the model area.

2. Longitude. If available this built-in constant returns the longitude of the model area.

3. Bed level. If available this built-in constant returns the altitude of the model area.

4. AD time step (AD_DT). This built-in constant returns the time step in seconds between every advection-dispersion calculation.

5. MIKE 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

4.6 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:

1. Water layer height. This forcing returns the spatial distance between layers (in metres). In one layered grid systems the water depth will be returned

2. Salinity. If available this forcing returns the salinity calculated in the hydrodynamic setup

3. Temperature. If available this forcing returns the temperature calculated in the hydrodynamic setup

4. 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

6. Water surface level. This forcing returns the water level calculated in the hydrodynamic setup

7. 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 metres 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

10. Vertical current speed. This forcing returns the vertical current speed in metres 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 metre) calculated in the hydrodynamic setup. Under normal conditions positive values

12. Bed area of grid cell

13. Flooded area of grid cell

14. 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

4.7   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:

1. Daynumber(Year,Month,Day). This function returns an integer between 1 and 365 representing the daynumber in year.

2. Arrhenius20(TemperatureCoefficient,Temperature). This function returns a temperature dependency based on the following Arrhenius expression:

$$f(a, b) = a^{(b-20)} \qquad (4.1)$$

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

$$f(a, b) = a^{(b-5)} \qquad (4.2)$$

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

$$f(a,b) = \left(\begin{array}{l} 14,65 - 0,0841 \cdot a + b(0,00256 \cdot a - 0,41022 + b \\ (0,007991 - 0,0000374 \cdot a - 0,000077774 \cdot b)) \end{array} \right. \qquad (4.3)$$

5. 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.

$f(sali,temp)$ =(exp(-173.4292+249.6339*(100/(temp+273.15))+143.3483*(log((temp+273.15)/100))-21.8492*((temp+273.15)/100)+sali*(-0.033096+0.014259*((temp+273.15)/100)-0.0017*pow((temp+273.15)/100,2)))/0.69997) (4.4)

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

$$Lassiter(a, b, c, d, temp) = b \cdot e^{a(temp - c)} \cdot \frac{d - temp}{d - c}^{a \cdot (d - c)}$$ (4.5)

7. MichaelisMenten1(Concentration,HalfsaturationConstant):

$$f(a,b) = \frac{a}{a + b}$$ (4.6)

8. MichaelisMenten2(Concentration,Constant):

$$f(a,b) = \frac{a^2}{a^2 + b}$$ (4.7)

9. ReverseMichaelisMenten(Concentration):

$$f(a) = \frac{1}{a + 1}$$ (4.8)

10. Sunrise(Year,Month,Day,Latitude,CorrectionForSummerTime)

11. Sunset (Year,Month,Day,Latitude,CorrectionForSummerTime)

12. LambertBeer1(SurfaceLight,LayerHeight,LightExtinctionCoefficient). This function estimates the light penetration in water column based on Lambert Beer expression. The light intensity in the top of each grid layer is returned.

13. LambertBeer2(SurfaceLight,LayerHeight,LightExtinctionCoefficient)This function estimates the light penetration in water column based on Lambert Beer expression. The light intensity in the bottom of each grid layer

is returned.

14. RelativeDaylength(Month,Day,Latitude). Returns a value for relative day-length. The value equals 1 at equinox (when day and night have same length).

4.8 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
3. Inaccurate initial concentrations
4. Inaccurate hydrodynamic setup
5. Limitations in the chosen MIKE ECO Lab process descriptions
6. Inaccurate calibration of coefficients in MIKE ECO Lab process equations
7. Wrong measurements
8. 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:

4.8.1 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

4.8.2 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

4.9 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, half-saturation concentrations and also universal constants such as gas constant and atomic weights.

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

4.10 Courant Number

4.10.1 General Description

The transport Courant (Peclet) number is defined as

$$C_{rU} = \frac{U \Delta t}{\Delta s}$$

(4.9)

where Δt is the time step, U the current speed in one direction and Δs the grid spacing in the direction corresponding to U.

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

Please Note: A more restrictive condition is that the Courant number based on the flux, C_{rF}, is less than 1. C_{rF} is defined for the horizontal directions as C_{rU} with U replaced by the quantity F/h, where F is the local horizontal flux and h is the height of the considered grid cell. Often – but not always - C_{rF} is nearly equal to C_{rU}. Care should be taken in models with large gradients. If criteria

$C_{rF} < 1$

is violated during a simulation, a warning is given in the log file.

4.10.2 Remarks and Hints

The final transport Courant number is calculated as the sum of the Courant number in all three directions. This sum must theoretically be below 1.0. However, this criterion may in many cases be violated for shorter or longer periods during a simulation. In order to allow the execution to proceed, MIKE 3 automatically subdivides the time step used in the advection-dispersion update into smaller parts as

$$\Delta t_{NEW} = \frac{\Delta t}{N_{AD}}$$

(4.10)

This subdivision is permitted until N_{AD} equals 15.

4.11 CPU Time

4.11.1 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 *Hydrodynamic Module, Reference Manual and Hydrodynamic Module, Examples* manuals.

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 varies with the number of advective state variables and MIKE ECO Lab equations to be solved. In addition to the MIKE ECO Lab equations, the hydrodynamic mass and momentum equations are solved. In stratified areas also equation(s) for salinity or/and temperature variations are solved. Similarly, k and k-ε turbulence formulations imply extra equations to be solved

4.12 Deposition Concentration

4.12.1 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, e.g. pollution from air.
- Soil Deposition, e.g. leaching from highly contaminated sea bed.

4.12.2 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".

4.12.3 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".

4.13 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.

4.14 Disk Space

4.14.1 General Description

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

4.14.2 System Generated Files

- A specification file in the pfs system (Parameter File Standard) containing the simulation specifications will be generated by the menu system. This ASCII file will be placed in your present working directory and have a file extension of **M3**. It will only take up approximately 2 Kbytes.

- A log file describing the model set-up, the statistics of the files used and created during the simulation and a message for each time step completed will be generated by the computational module. The file extension of this ASCII file, which will also be placed in your present working directory, is **log** and it will usually take up less than 1 Mbytes on the disk. It is recommended always to carefully inspect the **log** file after termination, abnormal or successful, of a simulation.

4.14.3 User Defined Output 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.

If you wish to calculate the disk space required for a single output data file the following formula can be used. The result is in bytes:

$$4 \cdot NCPTS^P \cdot \left(NVAR \cdot \left(\frac{N_{last} - N_{first}}{N_{frequency}} + 1 \right) + NSKP \right) \tag{4.11}$$

$$\cdot \left(\frac{J_{last} - J_{first} + 1}{J_{frequency}} \cdot \frac{K_{last} - K_{first} + 1}{K_{frequency}} \cdot \frac{L_{last} - L_{first} + 1}{L_{frequency}} \right)^{1-p}$$

$$+ NHEADER$$

where NVAR is the number of output variables, N denotes time steps, J denotes points in the x-direction, K points in the y-direction and L points in the z-direction. NCPTS is the number of computational (water) points in the output domain. This number is normally not known prior to a simulation, but in the **Bathymetry dialog,** the total number of computational (water) points per time step can be seen. The power p is 1 for type 3 data files, and zero otherwise. NSKP is the number prefix records in the data file and equals zero for type 0 data files, 1 for type 1 and type 2 data files, and 5 for type 3 data files.

NHEADER is 1052 for files written in the older ctx/dtx format, and may vary slightly from 1052 for files in the dfs (Data File Standard) system.

4.14.4 Remarks and Hints

Please note that MIKE 3 does not check whether or not you have enough free disk space for your requested output files. If the required disk space is too large, you should sub-divide your simulation period into smaller parts using the "hot start" facility, see Hot data.

4.15 Dispersion Coefficients

4.15.1 General Description

The transport equation for an advective state variable concentration c is formulated as:

$$\frac{Dc}{Dt} = \frac{\partial}{\partial x_j} \left(\delta_j \frac{\partial c}{\partial x_j} \right) + \text{SS}$$

(4.12)

where SS is the source/sink term and δ_j is the dispersion coefficient in the j-direction. You have three options:

- The dispersion can vary proportionally to the local effective eddy viscosity with the factor of proportionality being $1/\sigma_T$, the dispersion factor. σ_T is the Prandtl number. Values of σ_T greater than one imply that diffusive transport is weaker for the concentration c than for momentum.

- The dispersion coefficients can be specified as being proportional to the local velocity components in each grid direction, e.g. in the x-direction δ_x is proportional $|u|$.

- The dispersion coefficients can vary proportionally to the local current vector, i.e. there are separate dispersions in the longitudinal, the transverse and the orthogonal directions.

4.15.2 Specifying Dispersion Factors

In the **Dispersion dialog** you choose the dispersion variation for each of the state variables from the combo-box selection placed to the right of each state variables name.

In the **Dispersion dialog** you also give the factor of proportionality. You must also specify the dispersion limits, i.e. the limits within which the dispersion coefficients are allowed to vary, for each grid direction: Defining the dimensionless dispersion coefficient for direction j as

$$D_j = \frac{\delta_j \Delta t}{(\Delta s_j)^2}$$

(4.13)

where Δs_j is the grid spacing in the j-direction, it is for stability required that the sum of all three D_j is less than 0.5.

4.15.3 Recommended Values

A wide range of values for σ_T occurs in the literature. In many cases a value of 10 can be applied, corresponding to a dispersion factor of 0.1.

When the mixed Smagorinsky/k-ε turbulence model is applied, the temporally and spatially varying values of σ_T are calculated as an integrated part of the turbulence model, and a dispersion factor of 1 is recommended.

4.15.4 Remarks and Hints

A constant dispersion coefficient may be obtained by entering a positive value for the proportionality factor and setting all dispersion limits equal to the desired value (in m^2/s).

The above mentioned dispersion stability criterion often leads to a restriction, which yields a small time step due to a very fine vertical resolution, see Time Step *(p. 56)*. Therefore, it might advantageous to select an implicit scheme for the vertical dispersion. With an implicit dispersion scheme in the vertical direction and an explicit scheme in the horizontal direction the above mentioned dispersion stability criterion is replaced by the less restrictive criteria

$D_x + D_y < 0.5$

$D_z < 10$

4.16 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 $\quad x_n \quad$ to $x_{n+1} = x_n + h$

4.17 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.

4.18 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 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. 44)* is applied.

4.19 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.

4.20 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.

4.21 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.

4.22 Hot Data

4.22.1 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".

In addition to the information described in the Hot Data section in the HD Reference Manual the hot data includes all component concentrations.

4.22.2 Specifying the Hot Data

You specify that you wish to be able to continue the simulation you are about to execute from the Hot Start dialog in the Hydrodynamic Parameters section. In other words, you cannot specify separate hydrodynamic and MIKE ECO Lab hot data.

You specify that you wish to do a simulation as a continuation of a previous one by selecting **Hot start** in the **Bathymetry dialog**, and then writing the **name** of the hot data created earlier.

4.23 Initial Concentrations

A description of the starting concentrations is required for all the MIKE ECO Lab state variables in a simulation. There are 3 possibilities:

1. the starting concentrations can be set to a constant value used

2. the starting concentrations can be **Read from Type 2 Data File** if the state variable has one of the 2D scopes: WS, WB, SED.

3. the starting concentrations can be **Read from type 3 data file** if the state variable has the scope 'WC'. A type 3 data file covering the model area as defined through the bathymetry may be created from an *xyzv*-file (ASCII file containing positions and values) with the **Digitising** tool in the MIKE 3 Toolbox.

4.24   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. (This item also includes any AD Solver mass corrections.)

- Accumulated mass added/removed by MIKE ECO Lab processes

- Accumulated mass deviation (error) within polygon determined as the difference between the mass change and the transported, added and removed mass

- If the 'Section transports' switch is enabled in the Basic Parameters Dialog, one or more additional time series will be provided in the mass budget. These correspond to the transports through each lateral section of the mass budget polygon. Notice that the sum of the section transports equals the total transport over the lateral limits of the polygon

This means that for every state variable selected, five or more 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, file name 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 state variable multiplied by 10^6 m^3. This means that if the unit of the state variable is mg/l, the mass unit will be 10^9 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.

4.25 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)
4. 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()

4.26 Output Area

4.26.1 General Description

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 state variables 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. You therefore

have the option of saving multiple parts of output in the advection-dispersion module.

4.26.2 Specifying the Output Area

In the **M3 ECO Lab Result** menu 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 by writing the number of the output area you wish to edit and pressing return:

- First you specify the data file name and data title.

- Secondly 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, you could specify the area of interest only. The type of your 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.

- You specify the range of time steps to be saved and if every time step should be included or only every second, third etc.

- Finally, you choose the desired output items. You may include the velocity components as well as any of the MIKE ECO Lab state variables and additional MIKE ECO Lab output.

4.26.3 Remarks and Hints

One way of following the progression of your simulation is by following the number of time steps written in your output data files (or one of them). In most post-processing tasks you start by specifying the data 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.

4.27 Precipitation Concentrations

4.27.1 General Description

In applications where the rainfall is important for the flow, you can include precipitation in your simulation. Precipitation is included into the simulation on the Precipitation dialog under Hydrodynamic Parameters. You may describe the precipitation either as a constant value or as a time series (type 0 data file), which then is applied to the entire model area, or as a time series of maps (type 2 data file) in which case each grid point is assigned its own value. The precipitation rate is specified in mm/day. You can use the **Time Series Editor** or the **Grid Editor** tool to create your precipitation data.

You can also use the precipitation facility to include evaporation in your simulation. This is simply done by specifying a negative precipitation. However, in simulations with temperature variations the evaporation is calculated as part of the latent heat flux if the heat exchange option is selected. Thus you should be careful not to specify evaporation from both options.

4.27.2 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 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 concentration" will be used when the specified net-precipitation is positive. When the net-precipitation is negative, an evaporation concentration of value zero is applied.

4.27.3 Evaporation Concentrations

When evaporation occurs or when the net-precipitation is negative, the evaporation concentration is always zero.

4.28 Predefined MIKE ECO Lab Templates

DHI has a number of standard MIKE ECO Lab templates.

1. EU.ecolab: Eutrophication
2. 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

4.29 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.

4.30 Process Matrix

A process matrix show the interaction between state variables and processes. It is a simple way of getting an overview of all 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'.

4.31 Process Type

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

1. Transformation. This is for instance in situ degradation, production, of matter. This process type transforms matter at the spot, and can not move or transport matter

2. Settling. This process moves matter down the water column, and in mulitlayered grid systems the matter is moved from layer to layer.

4.32 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.

4.33 Reserved words

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

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

4.34 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 righthand side per time step.

$$k_1 = hf(x_n, y_n) \tag{4.14}$$

$$k_2 = hf\left(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right) \tag{4.15}$$

$$k_3 = hf\left(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}\right) \tag{4.16}$$

$$k_4 = hf(x_n + h, y_n + k_3) \tag{4.17}$$

$$y_{n+1} = y_n + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} - O(h^5) \tag{4.18}$$

4.35 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.

4.36 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 grid point.

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 grid point.

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 discretisation 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 grid point.

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 grid point. 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.

4.37 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

1. 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:

4.37.1 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:

1. 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.

4.37.2 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:

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

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

1. already defined 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 an auxiliary variable with spatial variation 'HORISONTAL_AND_VERTICAL' are:

1. 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'

4.37.3 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 'HORISONTAL' are:

1. already defined processes, auxiliary variables, constants, forcings with spatial variation 'NONE' or 'HORISONTAL'

2. already defined processes with spatial variation 'HORISON-TAL_AND_VERTICAL' with scope 'WS', 'SED', or 'WB'

3. state variables with scope 'WS', 'SED', or 'WB'

Legal arguments to an expression for a process with spatial variation 'HORISONTAL_AND_VERTICAL' are:

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

4.37.4 Derived output

Scope is not user specified for Derived Output, but spatial variation must be specified and the options are 'NONE', 'HORISONTAL', and 'HORISON-TAL_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:

1. 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:

1. 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'

4.38 Source and Sink

4.38.1 General Description

The effects of rivers, intakes and outlets from power stations, outlets from sewers, etc., can be included in a simulation. MIKE 3 distinguishes between three different kinds of sources:

- isolated source, a point where a certain amount of water is discharged into the model with a certain velocity, affecting both momentum and continuity equations,

- isolated sink, a point where a certain amount of water is discharged out of the model, affecting only the continuity equation, and

- connected source–sink pair, used for recirculation studies, the amount of water removed at the sink is re-entered at the source point with a specified velocity.

The sources and sinks are included in the hydrodynamic equations as described in the HD User Guide (see .

4.38.2 Specifying Sources and Sinks

In your model you can have up to a total of 300 sources and sinks, the location and strength of which you must specify in the Source and Sink dialog of the Basic Parameters section and the Source and Sink dialog of the Hydrodynamic Parameters section.

- You specify the source concentrations of the advective state variables under AD Transport Parameters of the **MIKE ECO Lab dialog**. These may be given as constants or as included in a type 0 data file. You run through all sources one by one. For isolated sources the absolute value of the component concentration is specified whereas for connected source-sink pairs the excess source concentration is specified. At sinks, the intake component concentration equals that of the ambient water.

4.39 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:

1. None
2. Horizontal
3. 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.

4.40 Standard vs nested MIKE ECO Lab module

4.40.1 General Description

The purpose of this section is to enable the user to use the Nested MIKE ECO Lab module of the MIKE 3 Flow Model. As most features in MIKE 3 Nested ECO Lab are identical to the features in the standard MIKE 3 ECO Lab module, this section only describes the nested facilities, and the user is referred to other sections for guidance on common aspects.

The MIKE 3 Nested ECO Lab updates both MIKE ECO Lab equations and the advection-dispersion equations simultaneously in a user defined number of dynamically nested grids, and runs concurrently with the nested hydrodynamic module.

The advantage of applying the nested grid facility compared to the standard method of using only one grid is mainly the reduced CPU time requirements. Typical applications of the advection-dispersion 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.

4.40.2 Nested Model Specifications

As the MIKE 3 Nested ECO Lab module runs concurrently with the MIKE 3 NHD module, the rules laid out in the HD User Guide should be followed.

Most advection-dispersion specifications are identical in MIKE 3 ECO Lab and MIKE 3 Nested ECO Lab, but a few comments regarding the differences are listed below:

- Initial concentration fields should be specified for each area.

- Deposition concentration fields should be specified for each area.

- Precipitation concentrations are specified for the main area only and are interpolated to the relevant sub-areas.

- Dispersion coefficients should be specified for each model area.

- Decay factors are common for all model areas.

- As in MIKE 3 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 start data input/output for/from a MIKE 3 Nested ECO Lab simulation must be specified for each model area. The relevant hot start data is found in/written to the corresponding hot start data files from the MIKE 3 NHD simulation, i.e. HD and MIKE ECO Lab hot start data are in the same files.

Time step

The time step to be used in a MIKE 3 Nested ECO Lab simulation is determined in the same way as in MIKE 3 Nested ECO Lab (based on the maximum transport Courant number). However, in the nested version it is necessary to calculate the transport Courant number within each model area (or bathymetry) 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).

The CPU time is proportional to the number of computational water points in all model areas (neglecting the "hidden" water points due to nesting).

NOTE: MIKE 3 Nested ECO Lab allows for automatic subdivision of the time step separately in each model area, see Courant Number *(p. 34)*.

4.41   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.

4.42   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:

1. 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

5. Numbers

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

See also Semantic Rules.

4.43 Temperature dependencies

4.43.1 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.

4.43.2 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.

4.43.3 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.

4.44 Time Step

4.44.1 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 horizontal grid spacing, Δx.

- Secondly you decide on the maximum allowed Courant number, C_r.

- Then you can determine the maximum time step, Δt_{max} , which can be used in the model from the definition of the Courant number:

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

(4.19)

where c is the celerity. The time step to be used in the model, Δt, can then be chosen as a "convenient" number not greater than Δt_{max}.

- Furthermore, you have to check that the criterion on the final transport Courant number is not violated, see Courant number. As you have not yet carried out the simulation you will have to make an estimate of the maximum current speeds occurring during the simulation. Note that even for small vertical velocities C_{rU} could be large due to the often very small vertical grid spacing.

- Finally, you should check that the dispersion criteria described under Dispersion Coefficients *(p. 38)* as well as the Dispersion coefficients and Eddy viscosity in the Hydrodynamic module are fulfilled.

Please Note: A more restrictive condition is that the Courant number based on the flux, C_{rF} , is less than 1. C_{rF} is defined for the horizontal directions as C_{rU} with U replaced by the quantity F/h, where F is the local horizontal flux and h is the height of the considered grid cell. Often – but not always - C_{rF} is nearly equal to C_{rU} . Care should be taken in models with large gradients. If criteria

$$C_{rF} < 1$$

is violated during a simulation, a warning is given in the log file.

Also 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 (multipla 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.

4.45 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.

4.46 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.

1. 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.

2. 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.

3. 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.

4.47   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
4. Nitrite
5. Phosphate
6. Faecal Coliform
7. Total Coliform*

See the 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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