MIKE 3 Flow Model FM

ECO Lab / Oil Spill Module

User Guide

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CONTENTS

1 About This Guide

1.1 Purpose

The main purpose of this User Guide is to enable you to use, MIKE 3 Flow Model FM ECO Lab Module, for applications involving ecological modelling.

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 co-operation between engineers and biologists is recommended. It is assumed that you are familiar with the Hydrodynamic and Transport modules of MIKE 3 Flow Model FM. 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 available from the MIKE Zero General Documentation Index:

MIKE ECO Lab, User Guide

It is assumed that you are familiar with the basic elements of MIKE Zero: file types and file editors, the Plot Composer, the MIKE Zero Toolbox, the Data Viewer and the Mesh Generator. An introduction to these are available from the MIKE Zero General Documentation Index:

MIKE Zero Pre- and Postprocessing, Generic Editors and Viewers, User Guide

Plot Composer, User Guide

MIKE Zero Toolbox, User Guide

1.3 General Editor Layout

The MIKE Zero setup editor consists of three separate panes.

1.3.1 Navigation tree

To the left there is a navigation tree showing the structure of the model setup file, and it is used to navigate through the separate sections of the file. By selecting an item in this tree, the corresponding editor is shown in the central pane of the setup editor.

1.3.2 Editor window

The editor for the selected section is shown in the central pane. The content of this editor is specific for the selected section, and might contain several property pages.

For sections containing spatial data - e.g. sources, boundaries and output - a geographic view showing the location of the relevant items will be available. The current navigation mode is selected in the bottom of this view, it can be zoomed in, zoomed out or recentered. A context menu is available from which the user can select to show the bathymetry or the mesh and to show the legend. From this context menu it is also possible to navigate to the previous and next zoom extent and to zoom to full extent. If the context menu is opened on an item - e.g. a source - it is also possible to jump to this items editor.

Further options may be available in the context menu depending on the section being edited.

1.3.3 Validation window

The bottom pane of the editor shows possible validation errors, and it is dynamically updated to reflect the current status of the setup specifications.

By double-clicking on an error in this window, the editor in which this error occurs will be selected.

1.4 Online Help

The Online Help can be activated in several ways, depending on the user's requirement:

- **F1-key seeking help on a specific activated dialog:**

  To access the help associated with a specific dialog page, press the F1-key on the keyboard after opening the editor and activating the specific property page.

- **Open the Online Help system for browsing manually after a specific help page:**

Open the Online Help system by selecting "Help Topics" in the main menu bar.

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. 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, see e.g.

http://www.waterforecast.com

The need for tailormade ecosystem descriptions is large, because ecosystems vary. The strength of this tool is the easy modification and imple-mentation of mathematical descriptions of ecosystems into the hydrodynamic models included in DHI Software.

The user can use predefined DHI supported MIKE ECO Lab templates, or can choose to develop his own model concepts. The module can describe dissolved substances, particular 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 and ecological processes together with 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

3.1   General

The hydrodynamic basis for the MIKE ECO Lab Module must be calculated using the Hydrodymamic Module of the MIKE 3 Flow Model FM modelling system.

If you are not familiar with setting up a hydrodynamic model you should refer to User Guide for the Hydrodynamic Module and the comprehensive step-by-step training guide covering the Hydrodynamic Module of MIKE 3 Flow Model FM. The user guide and the training guide (PDF-format) can be accessed from the MIKE 3 Documentation index:

MIKE 3 Flow Model, Hydrodynamic Module, User Guide

MIKE 21 & MIKE 3 Flow Model FM, Hydrodynamic Module, Step-by-Step Training Guide

A comprehensive training guide covering the MIKE ECO Lab Module of the MIKE 3 Flow Model FM modelling system is also provided with the DHI Software installation. The objective of this training guide is to show how to set up an advanced MIKE ECO Lab model. The training guide (PDF-format) can be accessed from the MIKE 3 Documentation index:

MIKE 3 Flow Model FM ECO Lab Module, Step-by-Step Training Guide

The purpose of this chapter is to give you a general check list, which you can use when working with environmental projects using the MIKE ECO Lab Module in MIKE 3 Flow Model FM.

The work will normally consist of the tasks shown in the diagram in Figure 3.1.

As the diagram illustrates there can be different ways to reach the solution of your project.

Some tasks are mandatory, such as:

- Project analysis: defining and limiting the MIKE ECO Lab model
- Data collection
- Set up and run the model
- Calibration
- Solution: Running the production simulations
- Solution: Presenting the results

Other tasks in your project are optional and depend on your choice: do you plan to create your own MIKE ECO Lab template or just use a predefined one? In some cases a predefined template covering your specific problem does not exist, and then a new MIKE ECO Lab template has to be developed. If you choose to develop your own MIKE ECO Lab template, your project will include the following additional tasks:

- Development of Hypothesis/Theory: Litterature study and formulation of equations
- Implementation of theory into a MIKE ECO Lab template using the MIKE ECO Lab editor

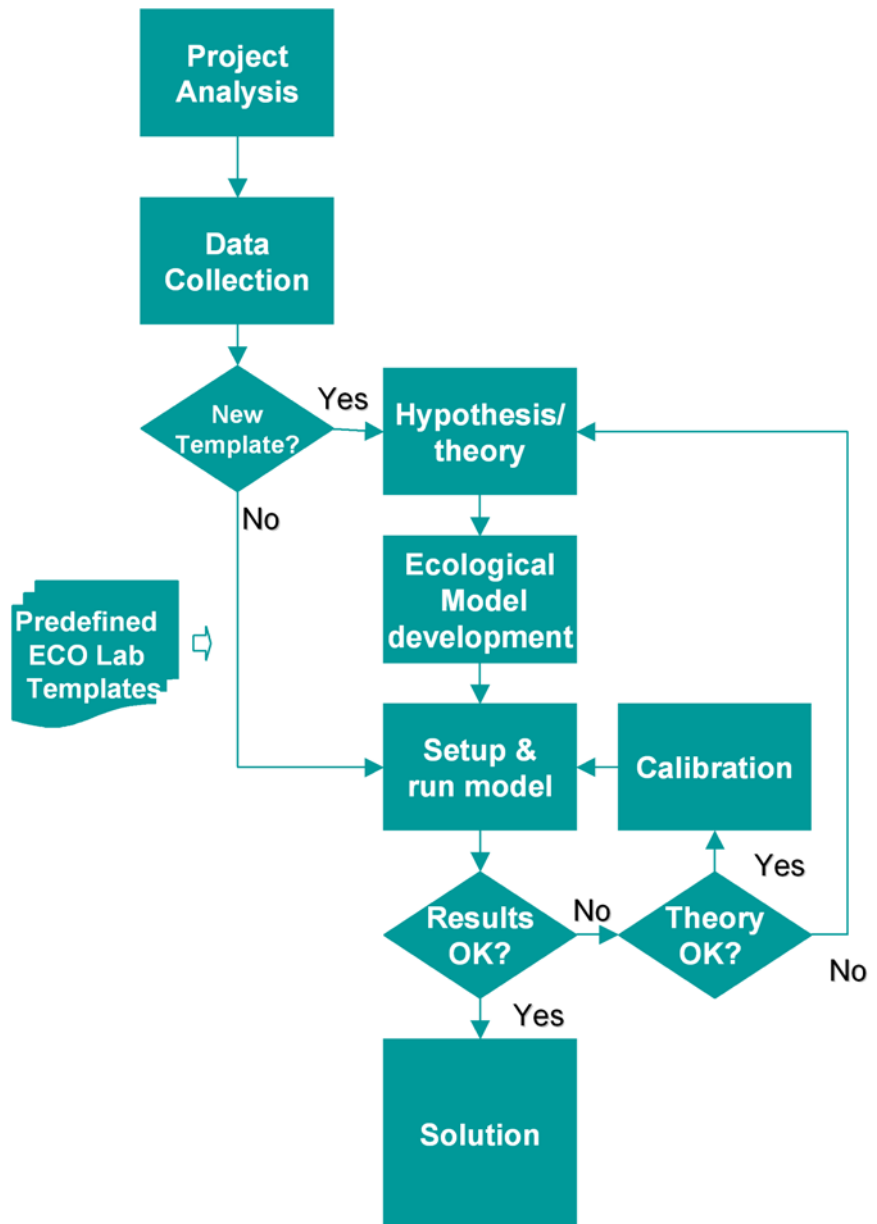Figure 3.1   Working with MIKE ECO Lab

You can see a list of available predefined MIKE ECO Lab templates in the MIKE Zero General Documentation Index.

3.2   Project Analysis

This task involves analysis and evaluation of the ecosystem problem and solution strategy. The considerations should be about:

1. What ecosystem state variables to simulate and the possible causal relations for their state. Describe which questions the model should be able to answer.

2. If it is possible at all to describe the ecosystem state variables with the available ecosystem knowledge, and if it possible to get sufficient data to simulate the state variables.

Figure 3.2   Illustration of the project analysis phase: Defining the problem and its causes and finding a solution strategy

The first thing to do is to point out the ecosystem variables that should be described with a MIKE ECO Lab model. In environmental projects these are often the variables that are considered as either dangerous, or vulnerable in the ecosystem. Also it is often seen that MIKE ECO Lab models should describe variables that are described in the criteria of environmental legislation. In aqua culture the state variables are usually those that affect the production.

The next thing to do is to point out the possible causal relations for the state of the system. The objective for most MIKE ECO Lab models is to be able to quantify these causal relations and their effect on the ecosystem. The best models tell us something that we do not already know even though we know the possible causal relation of a problem. For instance if an area has oxygen depletion, and experts agree that it is caused by eutrophication. Often they can not agree who is to blame for the anoxia. Are the nutrients imported from other areas and countries across the boundaries or are they coming from local effluents? A MIKE ECO Lab model describing eutrophication of the area would be able to give us such answers.

A MIKE ECO Lab model that describe the relation between cause and problem is also ideal for making prognostic scenarios. What happens to the oxygen concentrations in an area if we reduce the local nutrient loadings? A MIKE ECO Lab model describing eutrophication of the area would also be able to give us that answer.

Finally, the project analysis should involve development of a conceptual diagram of the ecosystem in question. It should be discussed if it is possible to

get adequate data and if enough ecosystem knowledge about the ecosystem exists to describe it.

3.3   Data Collection

This task involves the collection of data, field measurements and laboratory analysis and it may take a long time if you have to initiate a monitoring program. Alternatively it may be carried out very quickly if you are able to use existing data which are immediately available.

Figure 3.3   The phase of collecting data, e.g. field measurements and laboratory analysis

In all cases the following data should be collected:

- Bathymetric data such as charts from local surveys or, for example, from the Hydrographic Office, UK, MIKE C-MAP, etc.

- Hydrodynamic boundary data: Salinity, temperature, water levels and /or current velocities, which might be measurements or taken as model output from larger regional models

- Hydrodynamic forcings, for example wind, air temperature and clearness coefficient

- Hydrodynamic sources: Discharges from rivers and point sources

- MIKE ECO Lab boundary data: concentrations at the boundary of the advective state variables in the MIKE ECO Lab template, which might be measurements or taken as model output from larger regional models. Note that the frequency of measurements at the boundary can be very critical for the accuracy of the model

- MIKE ECO Lab forcings (depends on the content of the MIKE ECO Lab template), for example solar radiation

- MIKE ECO Lab loadings: Concentrations in sources and precipitation of the advective state variables in the MIKE ECO Lab template. The quality of these data is often very critical for the accuracy of the MIKE ECO Lab model. Make sure you have all the point sources and a proper assessment of the diffuse loading. Some times the loadings themselves are model output from e.g. MOUSE or MIKE 11. There are also DHI tools for estimating diffuse loadings that you might consider to use, if diffuse urban loadings are important in your MIKE ECO Lab study.

- MIKE ECO Lab initial conditions of MIKE ECO Lab state variables. If the retention time in the system is high, the initial conditions are quite important, and should be measured. If the retention time is low the initial conditions are not so important for the advective state variables, because the system quite fast will "flush" the system anyway, and the concentrations will be in balance after a short "warmup" period. Also the 'not-moveable' state variable (fixed) are often quite important to measure. Could for example be maps of benthic vegetation, benthic fauna etc.

- Calibration data; these might be measurements from different monitoring stations. They are used for comparing simulated values with measured values. So these data are important for documenting the capability and quality of the model.

3.4   New MIKE ECO Lab Template?

Is any predefined MIKE ECO Lab Template sufficient, or does the ecosystem that you want to describe require a dedicated MIKE ECO Lab template?

DHI has a number of predefined MIKE ECO Lab templates.

- Eutrophication MIKE ECO Lab templates

    These are predefined DHI supported MIKE ECO Lab templates that include models of eutrophication processes in aquatic systems.

    Eutrophication 1 is the classic DHI Eutrophication model. Eutrophication 1 can be used with an extended description of sediment and benthic vegetation. *Eutrophication 2* is a template that includes features such as diurnal DO variations.

    You have access to the scientific description of the different eutrophication templates from the MIKE Zero General Documentation index. It is also possible to view the pdf file directly from the MIKE ECO Lab template editor when the EU template is loaded.
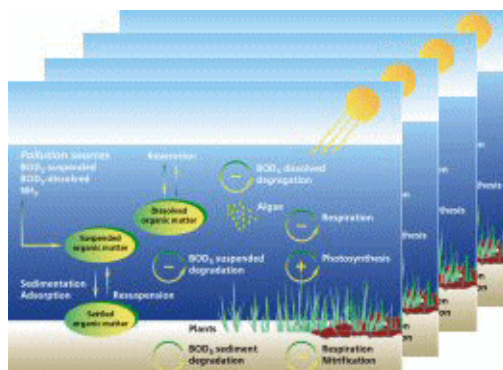
Figure 3.4   DHI has a number of predefined MIKE ECO Lab templates describing different types of ecosystems

- Heavy Metal MIKE ECO Lab template

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

  You have access to the scientific description from the MIKE Zero General Documentation index. It is also possible to view the pdf file directly from the MIKE ECO Lab template editor when the ME template is loaded.

- Water Quality MIKE ECO Lab templates

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

  State variables that are modelled with the WQ templates are:

  - BOD
  - DO
  - Nitrate
  - Nitrite
  - Phosphate
  - Faecal Coliform
  - Total Coliform

  You have access to the scientific description of the different water quality templates from the MIKE Zero General Documentation index. It is also possible to view the pdf file directly from the MIKE ECO Lab template editor when the WQ template is loaded.

3.5   Hypothesis / Theory

If none of the existing predefined MIKE ECO Lab templates cover your problem, you should formulate your own theories for your own template.

Describe in mathematical terms the processes that affect the state variables and how the state variables interact with each other.
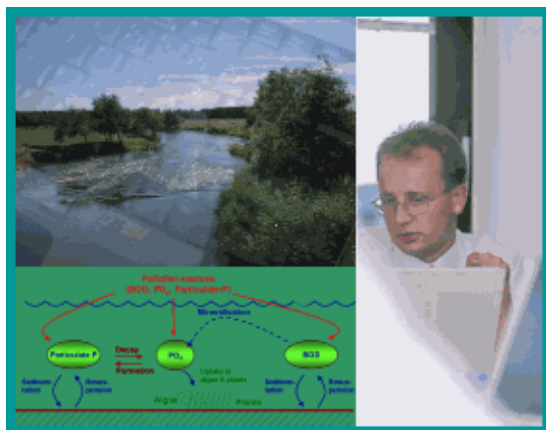
Figure 3.5   The mathematical formulation of theory for a new MIKE ECO Lab template usually requires a literature study

Ecosystem knowledge is usually collected by searching in literature.

3.6   Implementation of Theory in the MIKE ECO Lab Template

When you have formulated your mathematical description of an ecosystem, you should implement it in a new MIKE ECO Lab template. You create a new template with the MIKE ECO Lab editor and enter your expressions with the editor.
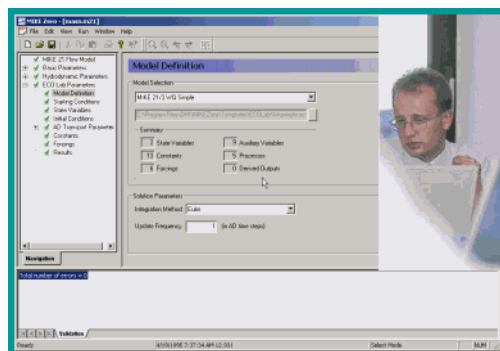
Figure 3.6   Implementation of ecosystem theory into a MIKE ECO Lab template is easy with the MIKE ECO Lab editor

See the User Guide for MIKE ECO Lab available from the MIKE Zero General Documentation index.

3.7   Set Up and Run Model

Whether you created your own template or you picked one of the existing templates, you are now ready to set up the MIKE ECO Lab model in MIKE 3 Flow Model FM.

Please see the step-by-step training guide for MIKE FM ECO Lab for learning how to set up an advanced MIKE ECO Lab model. This can be accessed from the MIKE 3 Documentation Index:

MIKE 3 Flow Model FM ECO Lab Module, Step-by-Step Training Guide

If you are not familiar with setting up a hydrodynamic model you should refer to the Step-by-step training guide for the Hydrodynamic Module:

MIKE 21 & MIKE 3 Flow Model FM, Hydrodynamic Module, Step-by-Step Training Guide

3.8   Calibration

By calibration of a MIKE ECO Lab set-up in any of the hydrodynamic models included in DHI software it is attempted to find the best accordance between computed and observed state variables (model components) by variation of a number of parameters.
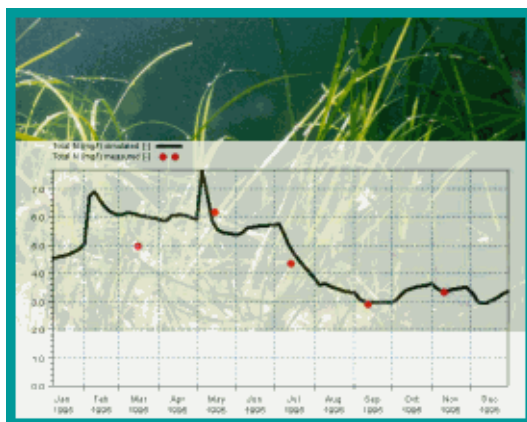
Figure 3.7   Calibration phase: adjusting the model so that the model output fits the measurements

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 set-up

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. Unstable numerical solution

The MIKE ECO Lab modeller should when calibrating a MIKE ECO Lab set-up have the above-mentioned possible reasons for inaccuracy in mind, before changing relevant 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.

If the output deviates from the measurements in a way that can not be accepted the user has to identify if the problem is caused by a wrong ecosystem theory, or if the reason is caused by another of the reasons mentioned above. Whether the template has to be changed or not, this calibration task will continue until the model describes the ecosystem in a causal way.

3.9 Solution

When the calibration is satisfying, the last task remains: Running the production simulations.

Now it is time to use the model and get answers from the model. Usually this task will include simulation covering different scenarios.

MIKE Zero includes a number of advanced plotting facilities, that are useful in this phase, when presenting your results. See the facilities in Plot Composer and MIKE Animator Plus.

4   Examples

Please see the step-by-step training guide for MIKE 3 Flow Model FM ECO Lab Module, for learning how to set up an advanced MIKE ECO Lab model using MIKE 3 Flow Model FM ECO Lab Module. The guide is available from the MIKE 3 Documentation index:

> MIKE 3 Flow Model FM ECO Lab Module,
> Step-by-step training guide

Further examples focusing on ABM modelling can be also be accessed from the Documentation Index:

> MIKE 3 Flow Model FM, ABM Lab - Drifter Example,
> Step-by-step training guide

To demonstrate the capabilities of Oil Spill modelling some examples are included with the installation of MIKE Zero. The directory names are as follows:

- Oil refinery (2D):
  .\Examples\MIKE_21\FlowModel_FM\ELOS\Refinery_OS

- Extended Oil spill template, surface spreading (2D):
  .\Examples\MIKE_21\FlowModel_FM\ELOS\Extended_OS

- Extended Oil spill template, Oil spill boom example (2D):
  .\Examples\MIKE_21\FlowModel_FM\ELOS\Extended_OS

The approach for oil spill modelling is similar for a 3D model.

4.1   Oil Refinery Example

4.1.1   Purpose

Prøvestenen is an artificial island that was originally created for the location of a fortress, whose mission was to protect the entrance to Copenhagen. In 1922 the area was converted to store oil and petrol. Today Prøvestenen offer the Copenhagen oil port for the reception of tankers. Prøvestenen harbour has a tank storage capacity of 1,000,000 m^3 for inflammable liquids.

In january 2008 a significant oil spill from Prøvestenen occured where several hundred thousand liters of Vacuum Gas oil ran out into the Sound. The accident happened when there was a hole in the hose to an oil tanker. The oil flowed north past Hellerup, Skovshoved up to Ven. Luckily, due to the low water temperature and the properties of the oil a large part of the oil could be picked up in clumps by environmental ships during the first 24 hours after the spill, but some of the oil drifted to settle on the coast between Helsingborg and Landskrona in Sweden.

With this accident in mind the Oil Spill model is setup to simulate the fate of different types of oil from an accident and to investigate the influence of water temperature on the weathering processes.The matrix of simulations is given in Table 4.1

Table 4.1   Combinations of climatic conditions and oil type

Oil type	Winter	Summer
Heavy fuel	SimA_1	SimA_2
Crude oil	SimB_1	SimB_2
Gasoline	SimC_1	SimC_2

4.1.2   Scenario

The hydrodynamic setup correspond to the setup described in the step-by-step training guide covering the MIKE 21 Flow Model FM. This guide is available from the MIKE 21 Documentation Index:

MIKE 21 & MIKE 3 Flow Model FM, Hydrodynamic Module, Step-by-Step Training Guide

The test conditions are:

- The sound area covers about 60 km x 100 km
- The simulation period for the oil spill is selected to 24 hours from midnight december 11th to midnight december 12th, during which the flow direction shifts after 12 hours. At the same time the wind shifts from south-westernly wind to northwesternly wind (see Figure 4.1).
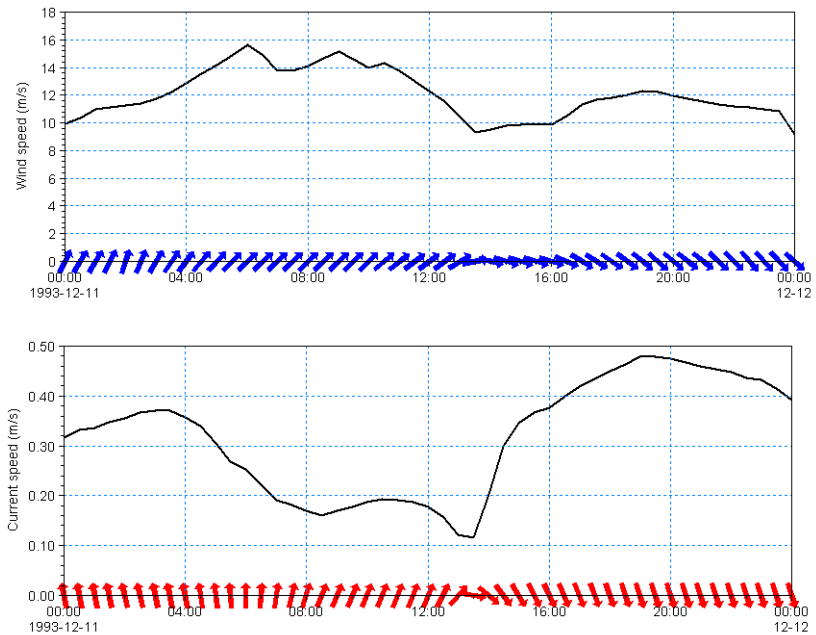
Figure 4.1   Descriptive conditions for oil spill simulation
Upper: Wind speed and direction
Lower: Simulated current speed and direction next to oil refinery

- The time step for the oil spill simulation is set to 300 s.

- The source spill event is simulated by a time-varying source positioned at the location of the oil refinery: 200 m^3 of oil was spilled during a 20 minutes period in the beginning of the simulation.

- Two water temperatures are investigated: winter conditions at 5 degrees Celcius and summer conditions at 15 degrees Celcius.

- Three types of oil are investigated: Heavy fuel oil, Crude oil (Statfjord) and Gasoline. The characteristics of each oil type are derived by the information given in the ESTC Spill Technology Databases[1].

4.1.3   Parameters HD simulation

The main condition defining the hydrodynamic problem is:

- The model area is resolved by an unstructured mesh with 3636 elements and 2057 nodes. The mesh is shown in Figure 4.8.

- An overall time step of 300 seconds is used and the duration of the HD simulation is one day starting at 11/12/1993 00:00:00.

- Initial flow conditions are derived from a previous HD simulation.

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1   http://www.etc-cte.ec.gc.ca/databases/OilProperties/oil_prop_e.html

- The south and north boundaries are each defined with water levels specified as line series

- The wind forcing is included as varying in time but constant in domain. The wind conditions are measured in Kastrup. The wind friction varies with the wind speed using default values.

- The eddy viscosity has been chosen to Smagorinsky formulation with a constant value of 0.24.

- The bed resistance type has been chosen as Manning number, with a constant value of 45 $m^{1/3}/s$

- Decoupled data files are output for future use.

- The resulting conditions (water level, total water depth and current conditions) are saved to an output file.
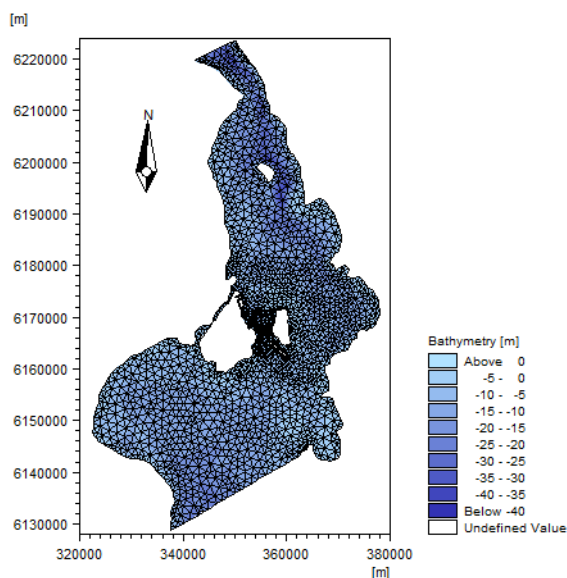
Figure 4.2   Model area, the sound between Denmark and Sweden

4.1.4   Parameters - OS simulation

The main settings defining the oil spill problem are:

- The processes for the oil spill are described by the Oilspill_A3, DHI Oil Weathering model, template.

- The derived oil properties for the different oil types are shown in Table 4.2 below..

Table 4.2   Oil properties for the three oil types in the simulations

	Heavy Fuel oil	Crude oil	Gasoline
Distribution in (%):			
Volatile oil	25	50	100
Heavy oil	47	40	0
Wax	2	8	0
Asphaltene	26	2	0
Distillation percentage at 180 deg.C	1	26	95
1st oil specific constant	-0.12	2.67	13.2
2nd oil specific constant	0.013	0.06	0.21
Simple evaporation type	1 (quad)	0 (log)	0 (log)
Density (kg/m^3)			
Average	1010	831	753
Volatile	755	755	753
Heavy	1094	907	-
Dynamic Viscosity (cP)	13460	6	1
Viscosity coefficient temperature dependency	-0.136	-0.111	0

- Other processes are defined by default values.

- The dynamic viscosity values are given at reference temperature 15 degrees Celcius.

- The source spill of this class is simulated for an event located at (E: 351600 N: 6173500) The position of the source is shown in Figure 4.9.
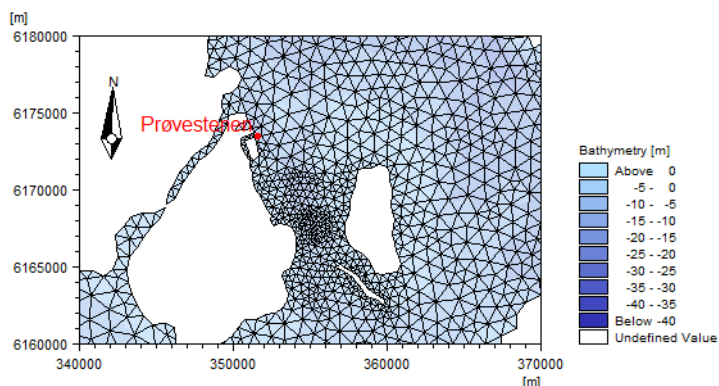
Figure 4.3   Location of Prøvestenen shown in detail of model area

- The 200 m³ of released oil corresponds to a total mass of each oil component as given in Table 4.3...

Table 4.3   Total mass for each oil component in the simulations

	Heavy Fuel oil	Crude oil	Gasoline
Distribution in (kg):			
Volatile oil	37750	75500	150600
Heavy oil	102836	72560	0
Wax	4376	14512	0
Asphaltene	56888	3628	0

- 60 particles are released per time step, corresponding to 25% of the oil particles.

- The mass values are interpreted as flux. Hence the mass values in Table 4.3 are divided by 1200 (20 x 60s) to obtain the flux values.

- The horizontal dispersion is included using a constant value in the dispersion coefficient formulation of 2.0.

- Vertical dispersion is not included

- The drift profile is defined by Surface Wind Acceleration with a wind weight of 0.02 and a wind drift angle of 15 degrees.

- The wind forcing is defined as in the HD simulation

- The influence of waves is omitted from the calculation

- The first output file is a dfsu file containing the state variables. The dfsu file is saved every 6 time step (30 minutes).

- The second output file is a Particle file (xml file) and will contain every 5th particle saved every 6 time step.

4.1.5   Results

The spill is released during the first 20 minutes of the simulation (4 time steps). The currents combined with the drag force from the westerly wind at the water surface may transport the oil away from the coast and out into Oresund in the beginning of the simulation. When the wind and current change direction the oil slick flows towards south. Figure 4.4 to Figure 4.6 shows the resulting particle tracks from the three simulations.

Figure 4.4   Particle tracks during simulation, Heavy Fuel oil type

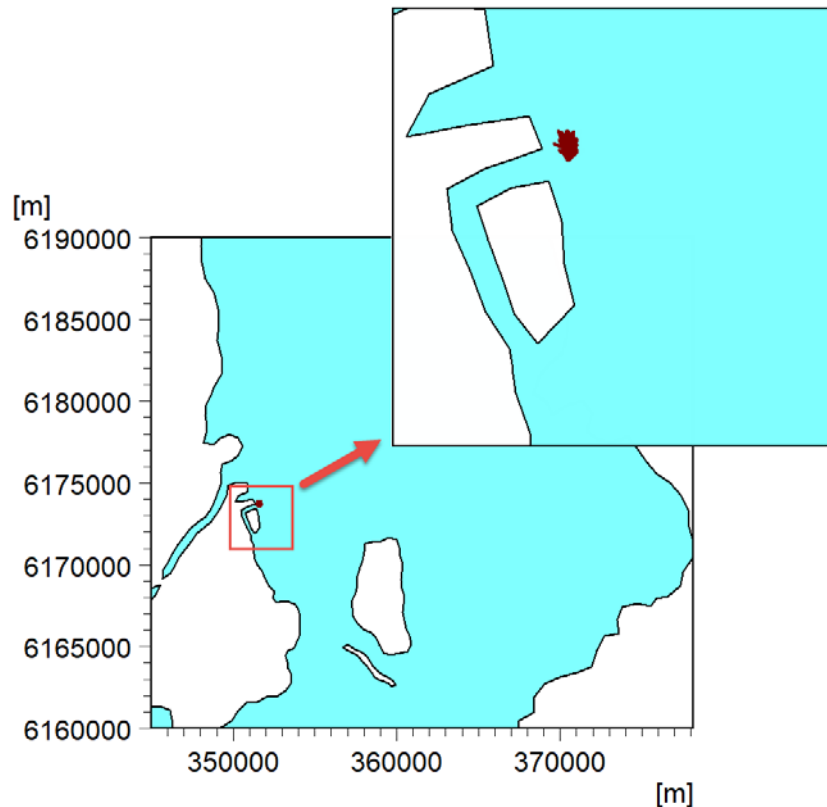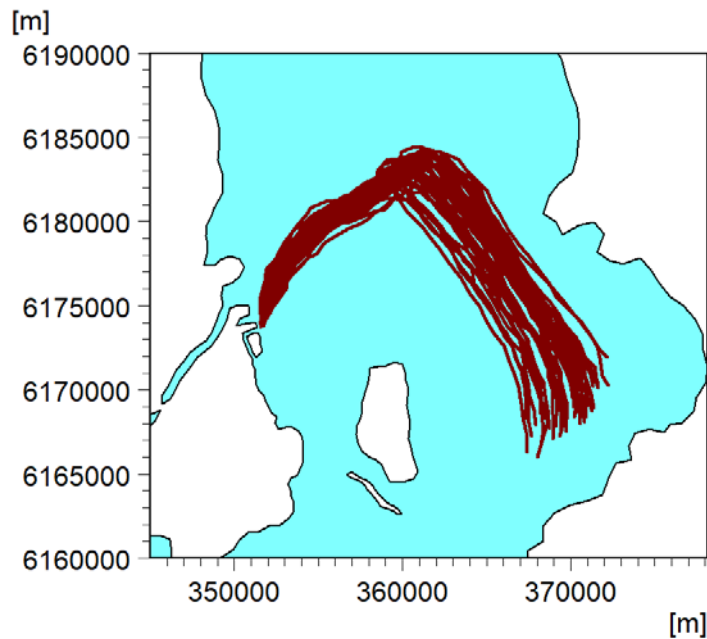Figure 4.5   Particle tracks during simulation, Crude oil type
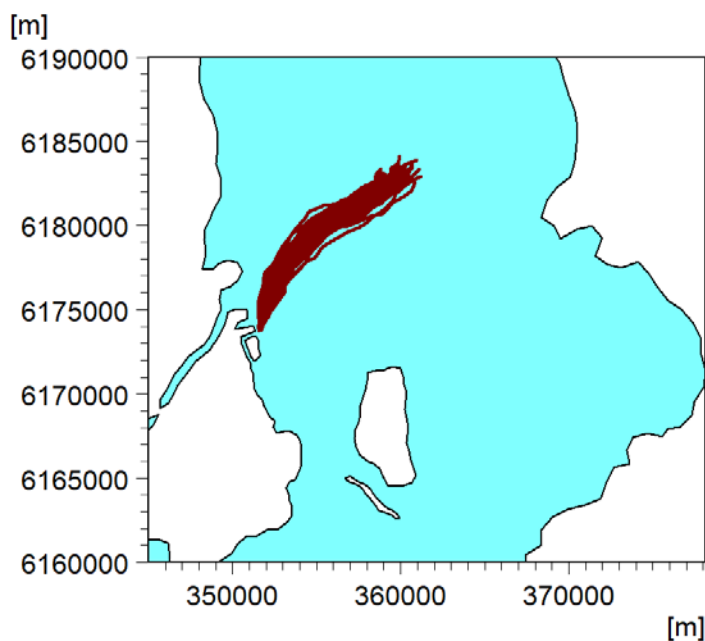
Figure 4.6   Particle tracks during simulation, Gasoline oil type

As seen from the three figures above the track is not the same for all the oil types. Some of the oil particles reach the bottom during the 24 hour simulation while others stay out into the water. And some particles evaporates

before the end of the simulation. This is because of the different composition of the oil types and the related difference in the weathering processes.The horizontal dispersion adds to the spreading of the results.

The evaporation of volatile material typically takes place during the first hours of an oil spill. To illustrate the process for this example, the Particle Track tool in the Oil Spill Particle Track toolbox has been used for extracting specific values from the XML files to dfs0 files. Figure 4.7 shows the total mass of the volatile components during the simulation for the three oil types, winter and summer, respectively.
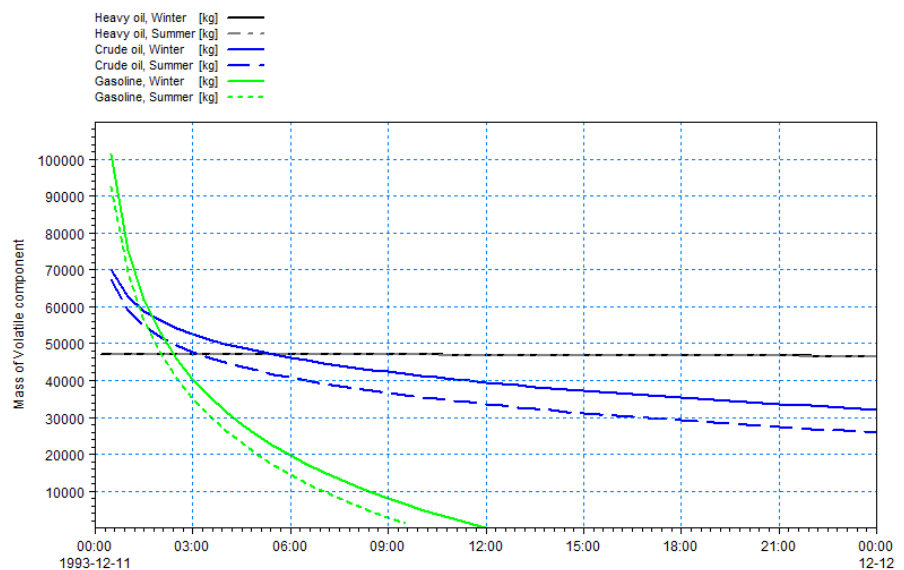
Figure 4.7   Mass of volatile components during simulation.

As seen from Figure 4.7 the volatile component of the oil quickly decrease during the first part of the simulation for the lighter oils. The oil evaporates more quickly in the summer than in the winter due to the higher temperature. The volatile component in Gasoline evaporates entirely during the simulation, whereas the evaporation rate for the volatile component of the Crude oil seem to decrease slightly after the first hour. This behaviour can be explained by weathering processes: as the oil density increase due to evaporation the oil becomes more viscous and evaporation is slower. The settling velocity changes and subsequently influence the movement of the particles. In the case of heavy oil the evaporation is very slow but this also relates to the fact that the heavy oil settles on the bottom very quickly, see Figure 4.8 and Figure 4.9.
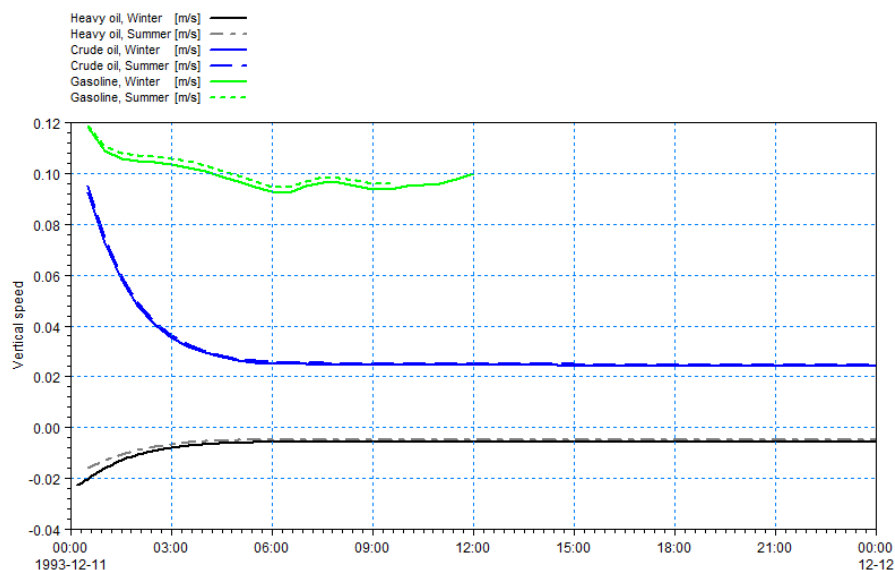
Figure 4.8   Vertical speed of oil particles during simulation.
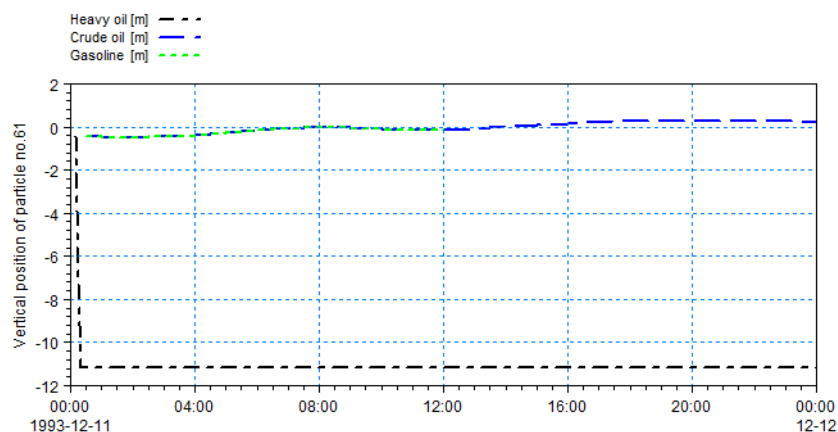
Figure 4.9   Vertical position of oil particle number 61 during simulation.

Figure 4.8 shows the vertical speed of the oil particles. This can be interpreted as a negative fall velocity. The lighter oil types remain buoyant during the simulation even if the oil particles becomes less buoyant as the lighter components evaporate. On the other hand the fall velocity for the heavy oil particles decrease as emulsion processes cause uptake of water into the oil particles.

As seen by Figure 4.9 the oil particles are released and the lighter particles remain at the water surface whereas the heavy oil type sink quickly towards the bed. When the oil particles are not at the water surface the evaporation

process is hindered and hence the volatile component of the oil particle remains constant, as seen in Figure 4.7.

By using decoupled files from a hydrodynamic simulation it is possible to speed up an oil spill simulation as the hydrodynamic flow is already calculated. This can e.g. be used to quickly assess the impact of changing various parameters.

The simulation of Heavy oil in winter is used as an example, where results for particle numbers 11, 71, 131 and 191 has been extracted and shown below. The oil spill specifications are changed such that it includes a vertical dispersion factor of 1, and the Drift profile is change to the type 'Use bed shear profile and surface wind acceleration'. The output is restricted to the first hour of simulation, but with output each time step.
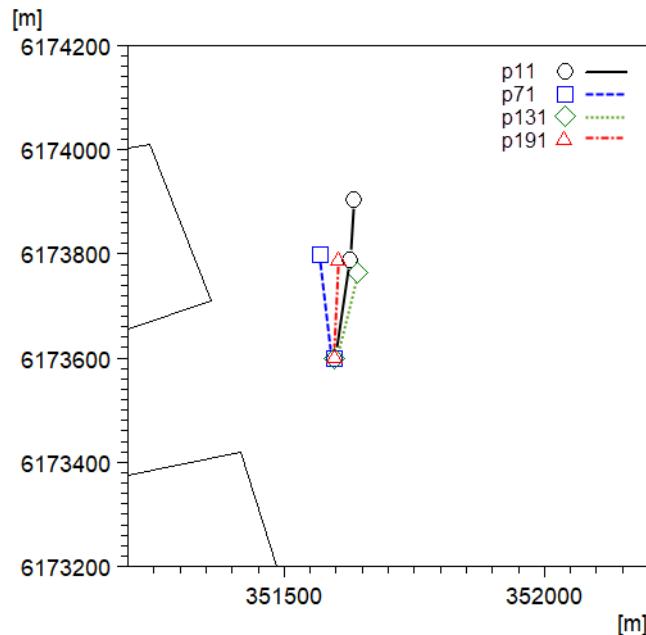
Figure 4.10   Heavy oil particle positions in domain for 4 specific particles

It can be seen from the figures that there are no larger impact from adding the vertical dispersion in this case. The heavy oil particles generally reach the bottom and settle within short time. Figure 4.11 and Figure 4.12 illustrates that even if the oil particles has settled on the bed, the processes continues and the water fraction of the oil particles will continue to increase until an upper limit is reached.
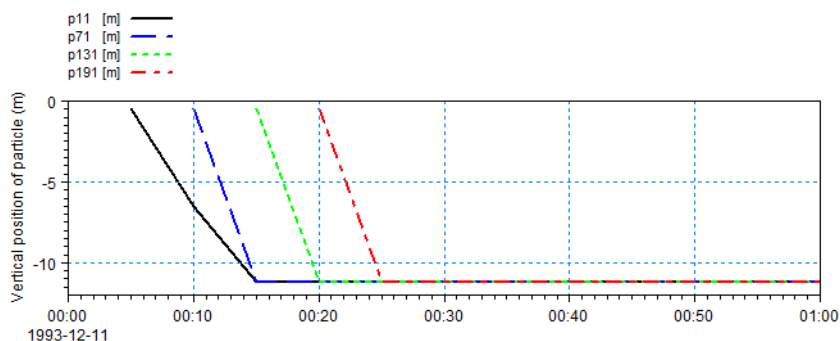
Figure 4.11 Vertical position of heavy oil particles during the first hour of simulation.
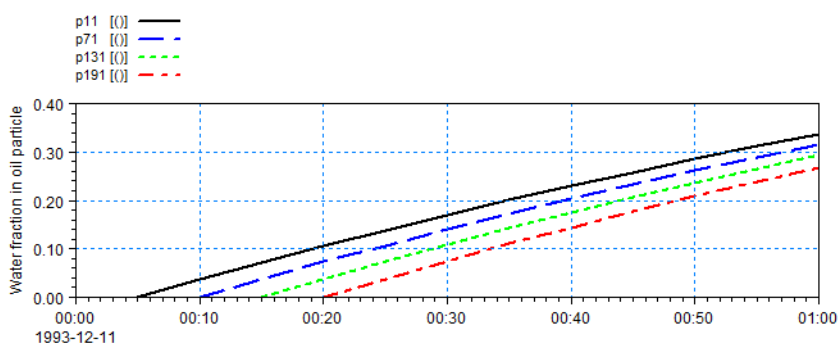
Figure 4.12 Content of water in heavy oil particles during the first hour of simulation

4.1.6 Files

The following data files (included in the \ELOS\Refinery_OS folder) are supplied with MIKE 21 Flow Model ELOS FM:

File name: SimHD.m21fm
Description: MIKE 21 Flow Model FM specification file. Contains the HD setup for generating decoupled files

File name: SimA1.m21fm, SimA2.m21fm
Description: MIKE 21 Flow Model FM specification files. Setups for Heavy oil, winter conditions and summer conditions, respectively.

File name: SimB1.m21fm, SimB2.m21fm
Description: MIKE 21 Flow Model FM specification files. Setups for Crude oil (type Statfjord), winter conditions and summer conditions, respectively.

File name: SimC1.m21fm, SimC2.m21fm
Description: MIKE 21 Flow Model FM specification files. Setups for Gasoline, winter conditions and summer conditions, respectively.

File name: SimA1_Decoupled.m21fm
Description: MIKE 21 Flow Model FM specification file. Setup for Heavy oil, winter conditions, using Flow conditions from decoupled files.

File name: ExtractParticleData.noilt
Description: Oil Spill Particle Track toolbox specification file

File name: OilSpill_A3.ecolab
Description: MIKE ECO Lab template for Oil Spill

File name: OilRelease.dfs0
Description: Contains state variables for oil source

File name: oresund.mesh
Description: Mesh file including mesh and bathymetry

File name: wind_kastrup.dfs0
Description: Wind speed and direction for area

File name: waterlevel_north.dfs1
Description: Water level variation at north boundary

File name: waterlevel_south.dfs1
Description: Water level variation at south boundary

File name: InitialFlowField.dfsu
Description: Initial flow field for HD simulation

4.2   Extended Oil spill template, surface spreading

4.2.1   Purpose

This example demonstrates the surface spreading of the oil particles in the extended oil spill template. The extended template contains a mechanism that ensures that oil particles are placed without overlapping if possible. Please note that this spreading is independent on the surface spreading of the oil itself (gravity spreading), i.e. simulated surface area of individual oil particles will change due gravity spreading until a terminal thickness is reached. Weathering process may further change a particles area due to changes in the oil mass represented by a particle. The overall area covered by all particles of the spill will be the result of the gravity spreading of the individual particles and the demonstrated mechanism of spreading the particle swarm to ensure no overlap of particles. An upper limit of the overall area covered by all particles will be the sum of the individual particles surface area if no overlap occurs.

4.2.2 Scenario

The scenario is a fully artificial, hour glass shaped water body (two 2x2 km basin connected by a narrow channel) of total 5x2 km and a constant water depth of 10 m. An initial oil spill is released at the centre of the west basin in the first time step. As there is no current movement, any large-scale movement of oil particles is driven by wind drift. To allow the oil particles to spread undisturbed wind first starts to blow from West in the second half of the simulation period. Wind drift parameters are tuned to ensure a strait drift towards East. Most oil weathering process are switched off as this simulation shall only demonstrate the surface spreading mechanism.

4.2.3 Parameters

To demonstrate the surface spreading of oil particles most weathering process are switched off by setting the relevant class constants of the "Oil" class to zero as shown in Table 4.4 below:

Table 4.4   Weathering process parameters in Extended Oil Spill template

Name	Description	Unit	Value
Enable_WaveDispersion	Vertical wave induced dispersion: on-off switch (0=off, 1=on)	logic switch (0/1)	0
Enable_EVAP	Evaporation: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_BIOD	Biodegradarion: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_PHOT	Photo-oxidation: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_Diss_s	Surface dissolution: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_Diss_wc	Water column dissolution: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_Wateruptake	Water uptake: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_Waterrelease	Water release: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_Diameterchange	Dropplet diameter change: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_Areachange	**Area change: on-off switch (1=on, 0=off)**	**logic switch (0/1)**	**1**
Enable_Boom	Boom handling: on-off switch (1=on, 0=off)	logic switch (0/1)	0

Table 4.4   Weathering process parameters in Extended Oil Spill template

Name	Description	Unit	Value
Enable_Dispergent	Dispergent handling: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_In_Situ_Burning	In-Situ burning handling: on-off switch (1=on, 0=off)	logic switch (0/1)	0

The surface spreading is controlled by the parameters listed in Table 4.5:

Table 4.5   Factors controlling the surface spreading

Name	Description	Unit	Value
ShuffleSpeedFactor	Disc spreading speed factor	undefined	300
rfak	Factor for area search function	undefined	3

The "ShuffeSpeedFactor" controls the speed overlapping oil particles move apart. In principle two overlapping particles will move apart from each other along the line connecting the centres of the particles. The overall speed is proportional to the overlap area and modified by the "ShuffeSpeedFactor"; lower values will cause a faster movement whereas higher values a lower speed. If unrealistic spreading patterns are observed, the "ShuffeSpeedFactor" should be adjusted, i.e. if insufficient spreading is detected the value should be lowered whereas with too much spreading[1] the value should be increased. The value is sensitive for the overall simulation time step and should be revisited when timing changes are done.

The "rfak" value influences which particles are tested for overlap. The surface spreading tests the neighbouring particles which centres that are more than "rfak * own_radius" away. The factor should only be modified if oil particles of quite different size interact (fx. particles from different spill events).

4.2.4   Results

Visualising surface spreading
To visualise the spreading effect the particle track is shown as an overlay over the dfsu output. The style settings shown in Figure 4.13 are applied to the instantaneous particle overlay.

---

1   In extreme cases a too fast spreading will result in an oil "ring" around the geometric centre of the particles
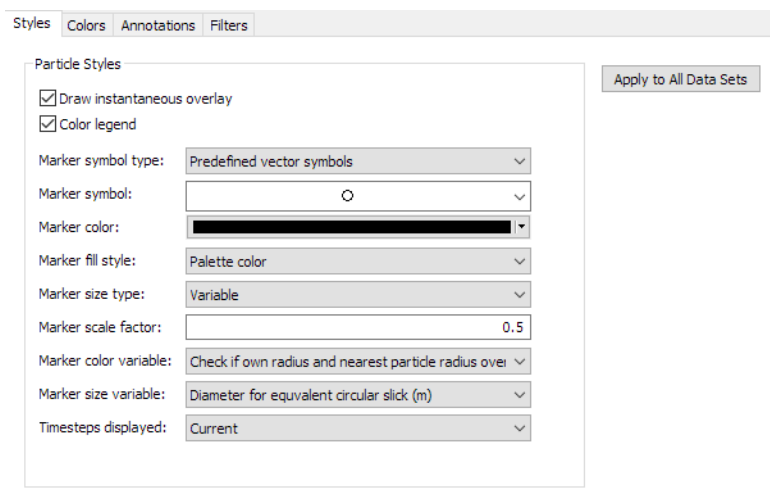
Figure 4.13   Style for visualising the particles

The oil particles are visualised as circles ("Marker Symbol") with a variable size ("Marker size type"). The size is derived from the oil particle variable "Diameter for equvalent circular slick(m)" with a scaling factor of 0.5 ("Marker scale factor").

To visualise the spreading speed the variable "Check if own radius and nearest particle overlap" is used to derive the particle colour. In real simulations one would probably use another property like the oil mass or thickness etc.

Shortly after the spill the oil particles are staged over each other and occupy a small area (see Figure 4.14). The dark blue colour of the particles represents a high overlap, particles with no overlap stress will appear red.
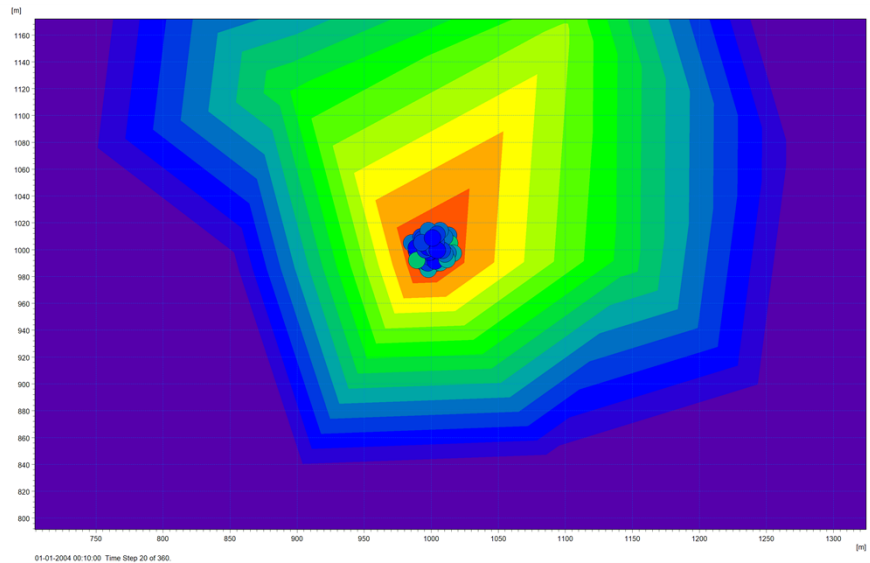
Figure 4.14   Particles shortly after the spill, time step 20
               Background contours illustrates concentration

Some time into the simulation the surface spreading has caused the oil parti-
cles to move apart (see Figure 4.15). The border particles show much less
overlap compared to the particles at the centre of the spill. Please note that
just a very gentle dispersion is used no other movement due to currents or
wind is active yet.
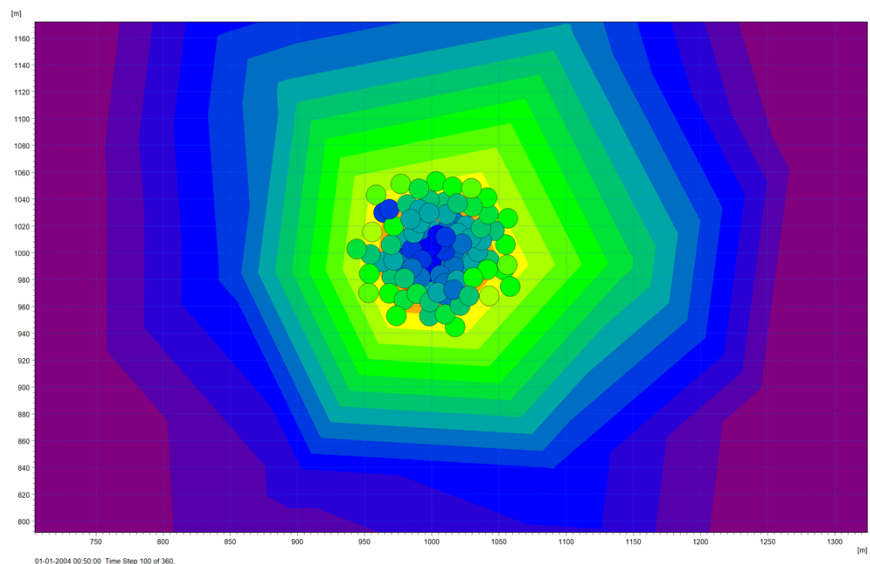
Figure 4.15   Particles some time into the simulation, time step 100

Directly before the wind sets in the oil slick has spread so much that there is very few overlap in the oil particles (see Figure 4.16).
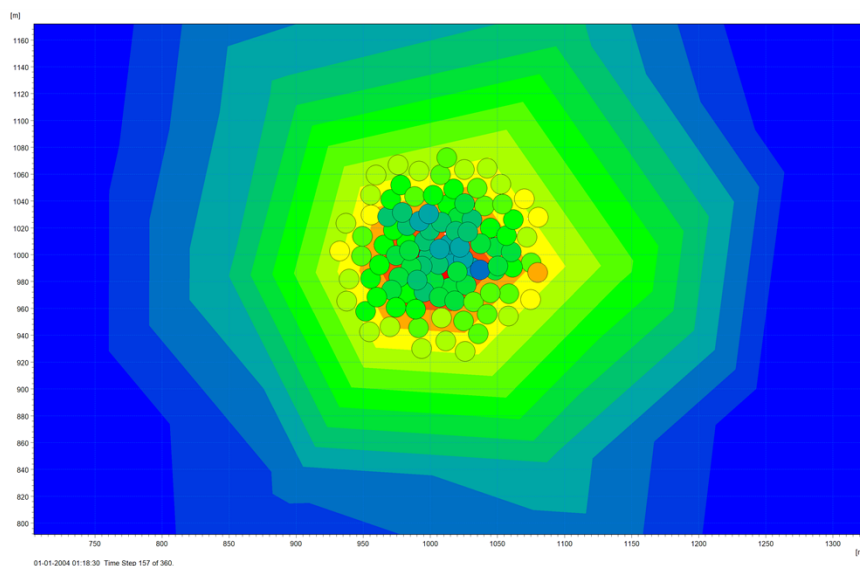
Figure 4.16   Particles just prior to the wind begins to affect movement, time step 157

When the wind sets in the whole spill moves East (see Figure 4.17). Note that the overlap in particles is even more reduced.
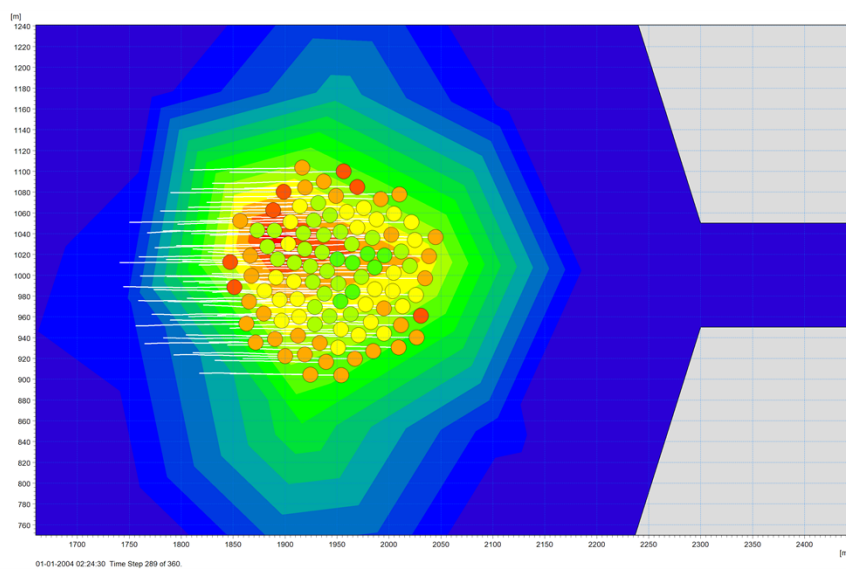
Figure 4.17   Particles when wind has set in, time step 289

When the wind pushed the oil spill into the channel some particles are blocked and accumulate at the shore (see Figure 4.18). This causes a high overlap detection.
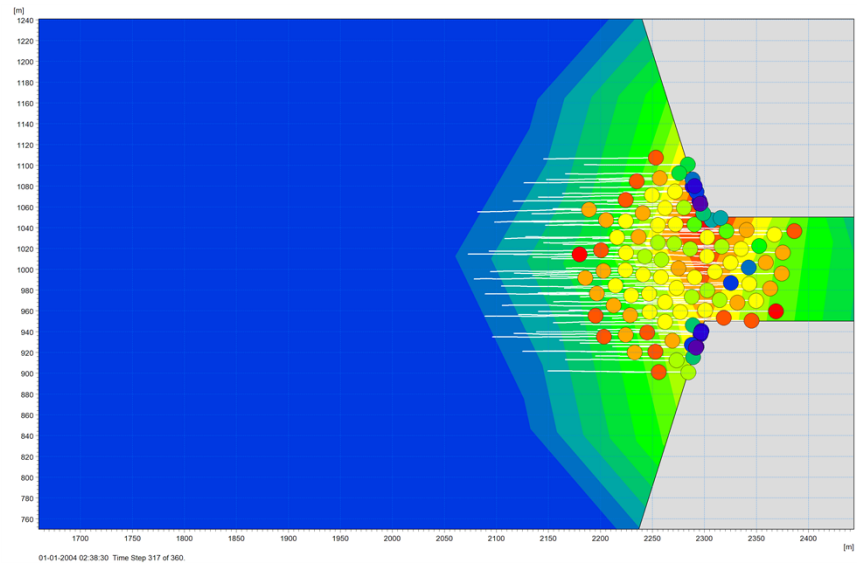
Figure 4.18   Particles when channel has been reached, time step 317

Effect of the "ShuffeSpeedFactor"

The following figures represent the effect of the "ShuffeSpeedFactor" value. In Figure 4.19 the factor is quite low and an artificial "ring" spreading pattern can be observed in the 2nd step
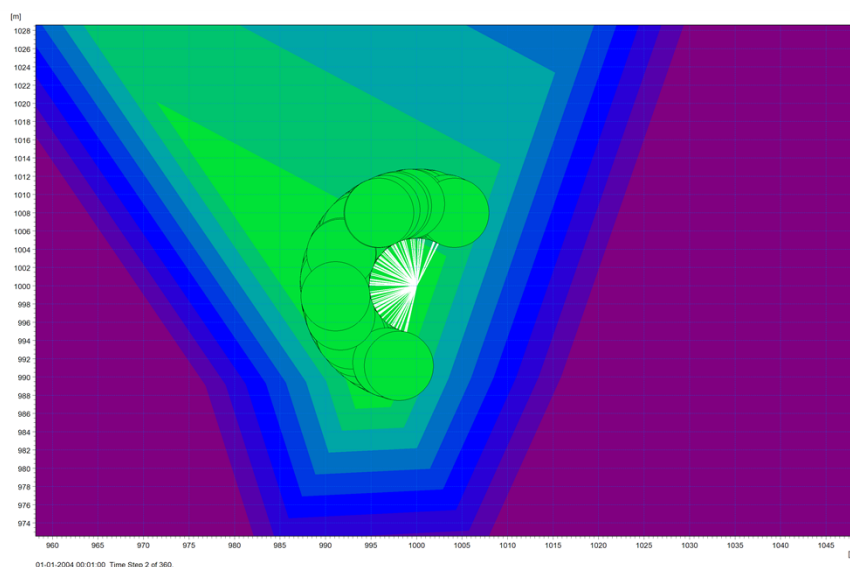
Figure 4.19   Low ShuffleSpeedFactor, particles in step 2

After 100 timesteps the particles are spread over a large area and show some "unnatural" jumping (compared to the corresponding image in Figure 4.15).
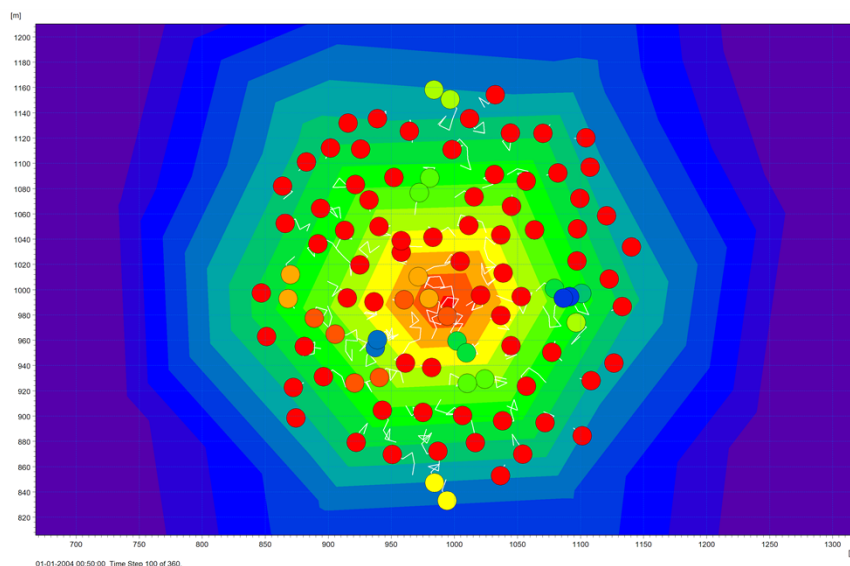
Figure 4.20   Low ShuffleSpeedFactor, particles in step 100

In the following figures the spreading factor was set to a high value. Consequently, the particles are not spread much at time step 100, see Figure 4.21.
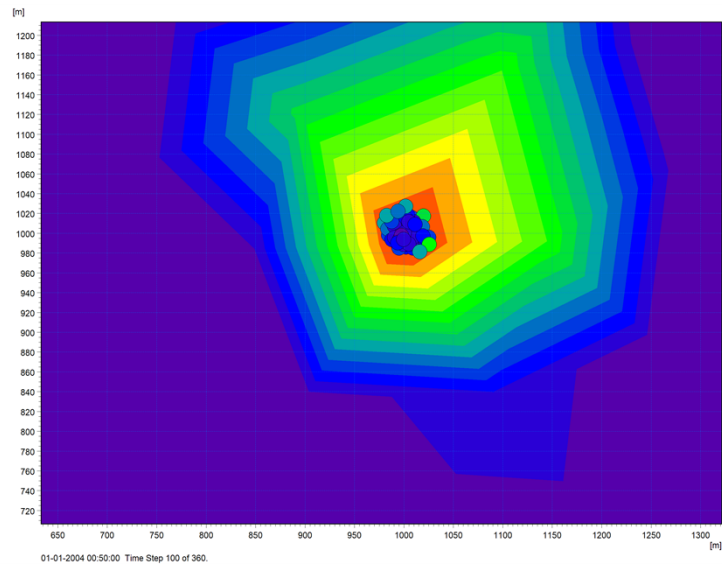
Figure 4.21   High ShuffleSpeedFactor, particles in step 100

Also, later in the simulation the particle swarm does not spread much and reaches the channel with a large overlap in all particles (see Figure 4.22). It almost passes the channel "en bloc"
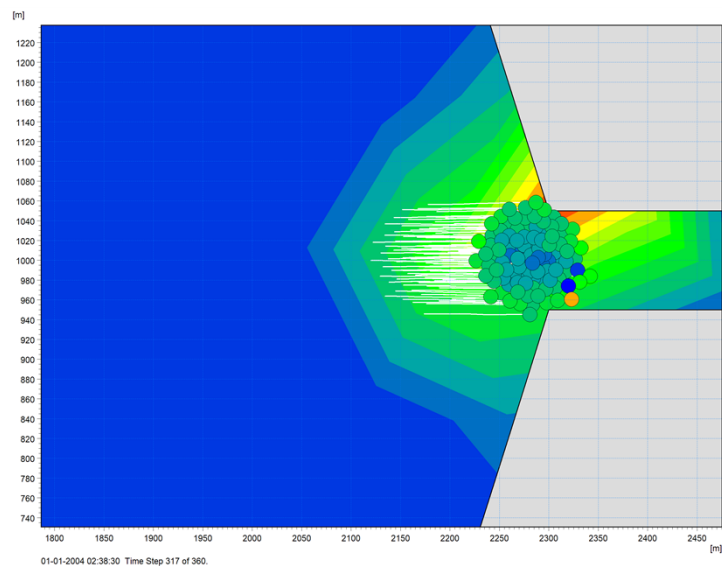
Figure 4.22   High ShuffleSpeedFactor, particles in step 317

4.2.5 Files

The following data files (included in the \ELOS\Extended_OS folder) are supplied with MIKE 21 Flow Model ELOS FM:

Filename: hourglass.mesh
Description: Mesh file including the mesh and bathymetry

Filename: Oilspill_Extended.ecolab
Description: copy of extended oilspill template (ECO Lab Template)

Filename: SurfaceSpreadingExample.m21fm
Description: MIKE 21 Flow Model FM specification file

Filename: WindSpeed.dfs0
Description: Wind data used in simulation

4.3 Extended Oil spill template, boom example

4.3.1 Purpose

The extended template contains a mechanism that simulates the application of containment and diversion oil booms. This example demonstrates how to define and use a boom to block the surface drift of oil particles in the extended oil spill template.

4.3.2 Scenario

The scenario is a full artificial, hour glass shaped water body (two 2x2 km basin connected by a narrow channel) of total 5x2km and a constant water depth of 10 m. An initial oil spill is released at the centre of the west basin in the first time step. As there is no current movement, any large-scale movement of oil particles is driven by wind drift. To allow the oil particles to spread undisturbed wind first starts to blow from West in the second half of the simulation period. Wind drift parameters are tuned to ensure a strait drift towards East. Most oil weathering process are switched off. It is basically the same scenario used in the surface spreading example described on page 39.

4.3.3   Parameters

To demonstrate the use of a boom definition to block the spreading of oil particles most weathering process are switched off by setting the relevant class constants of the "Oil" class to zero as shown in Table 4.6 below:

Table 4.6   Weathering process parameters in Extended Oil Spill template

Name	Description	Unit	Value
Enable_WaveDispersion	Vertical wave induced dispersion: on-off switch (0=off, 1=on)	logic switch (0/1)	0
Enable_EVAP	Evaporation: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_BIOD	Biodegradarion: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_PHOT	Photo-oxidation: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_Diss_s	Surface dissolution: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_Diss_wc	Water column dissolution: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_Wateruptake	Water uptake: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_Waterrelease	Water release: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_Diameterchange	Dropplet diameter change: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_Areachange	**Area change: on-off switch (1=on, 0=off)**	**logic switch (0/1)**	**1**
Enable_Boom	**Boom handling: on-off switch (1=on, 0=off)**	**logic switch (0/1)**	**1**
Enable_Dispergent	Dispergent handling: on-off switch (1=on, 0=off)	logic switch (0/1)	0
Enable_In_Situ_Burning	In-Situ burning handling: on-off switch (1=on, 0=off)	logic switch (0/1)	0

To simulate containment and diversion oil booms a special data file ("boom_-file.csv") must be present in the simulation root folder. This text file contains the definition of the boom nodes and line segments as well as the skimmer pump capacity over time. This means that the boom position can be adjusted/moved throughout the simulation.

The easiest way to produce a valid boom data file is to utilise the special "Oil-spill Boom and Skimmer" tool in the Oil Spill Particle Track toolbox. This tool allows to define the boom position and features using a graphical input editor.

When run the tool interprets the user input and generates a proper boom data file.

In general, the data file is a plain text file. All data is separated by a comma. After a header line at least one or multiple data definition lines follow. A data line describes the position of one or more boom segments at a time step.

The header line consists of 4 integer digits, **ndata, max_seg, utm_zone, projection**, as outlined in Table 4.7.

Table 4.7   Parameters in headline of ascii boom file

Variable	Description
ndata	Total number of data lines in the file
max_seg	Max number of segments defined in any data line
utm_zone	Local UTM zone used for coordinates if not using model zone
projection	Flag if model coordinates are UTM or long/lat (projection=1 'model is in UTM and local utm zone is the same projection=0 'model is in long/lat and coordinates are specified in local utm zone coordinates)

Each data line consists of a time stamp, the number of boom segments in the line and one or more boom segment definition. No more than **max_seg** segment definitions may occur in a data line!

{Timestamp}, NSeg, {boom segments}

A timestamp consists of 6 integer digits: **YYYY, MM, DD, HH, MM, SS**

Table 4.8   Parameters in time stamp

Variable	Description
YYYY	Yeat in 4 digits
MM	Month number (1=January, 12=December)
DD	Day number in month (1-31)
HH	Hour (0-23)
MM	Minutes (059)
SS	Seconds (0-59)

After the timestamp the number **NSeg**, i.e. the number of boom segment definitions in the data line follows. Each of these boom segments is defined by 7

numbers, **AX, AY, BX, BY, Pump_ID, Pump_capacity, Lock_prob**, as described in Table 4.9 below.

Table 4.9   Parameters for boom segments

Variable	Description
A_x	X coordinate of the segment start node A
A_y	Y coordinate of the segment start node A
B_x	X coordinate of the segment start node B
B_y	Y coordinate of the segment start node B
Pump_ID	ID of pump associated with the current line segment (1-n, integer number)
Pump_capacity	Capacity (in kg) of the pump (float number)
Lock_prob	Probability of any oil particle being locked/catched by the boom (0-1.00 = 0-100%) in a time step (float number)

The use of individual segments allows the definition of spatial independent booms.

A boom always floats on the surface and extends down into the water column. The boom thickness can be set in the template constant "BoomDepth" and is 1 m by default. Oil particles passing the surface below the boom are not affected.

The template constants outlined in Table 4.10 control the boom efficiency and effects.

Table 4.10   Template constants affecting boom efficiency and effects

#	Description	Default	
11	Maximum windspeed (m/s) for boom operation	0	m/s
12	Efficiency of skimmer pumps during daytime operation	100	%
13	Efficiency of skimmer pumps during nighttime operation	80	%
14	Wave height below no leakage from booms is observed	2	m
15	Wave height where booms become ineffective due to wave action	4	m
16	Minimum boom towing speed through water	0.05	m/s
17	Maximum boom towing speed through water	0.4	m/s
18	Viscosity where boom leakage due to low viscosity stops	0.5	cP
19	High viscosity limit in booms before leakage	0.7	cP

Table 4.10   Template constants affecting boom efficiency and effects

#	Description	Default	
20	A reduction factor in boom effectiveness at high Viscosity	0.2	Fraction
21	Minimal oil slick thickness before skimmer pumps become ineffective	0.1	mm
22	Boom Depth	1	m

Take care that these constants are set properly (especially #11, #16, #17 and #22), otherwise unexpected results (ineffective boom) may be observed.

Using the Oilspill Boom and Skimmer tool

To generate the boom definition file one can use the "Oilspill Boom and Skimmer" tool. If this tool is invoked the user has to provide a valid tool setup name for the tool as shown in Figure 4.23.
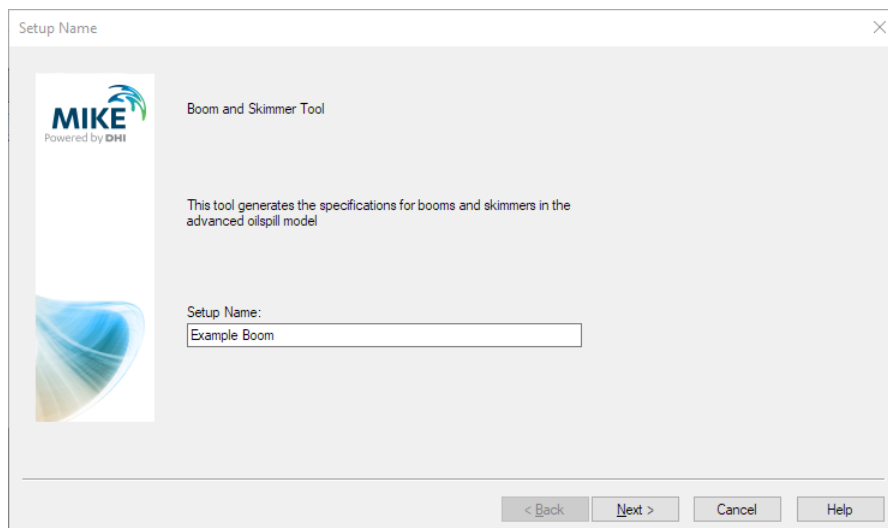
Figure 4.23   Intiial setup dialog for Boom and Skimmer tool in Oil Spill / Particle Tracking toolbox

On the following dialog the domain can be either read from a mesh file or be imported from an existing setup.

Figure 4.24   Dialog for specifying domain area for computation

When importing from a setup the time step settings are also imported to match the setup data. Otherwise the user has to provide a proper time step setting.

Figure 4.25   Dialog for specifying time for simulation

Now the user can place one or several booms in time and space
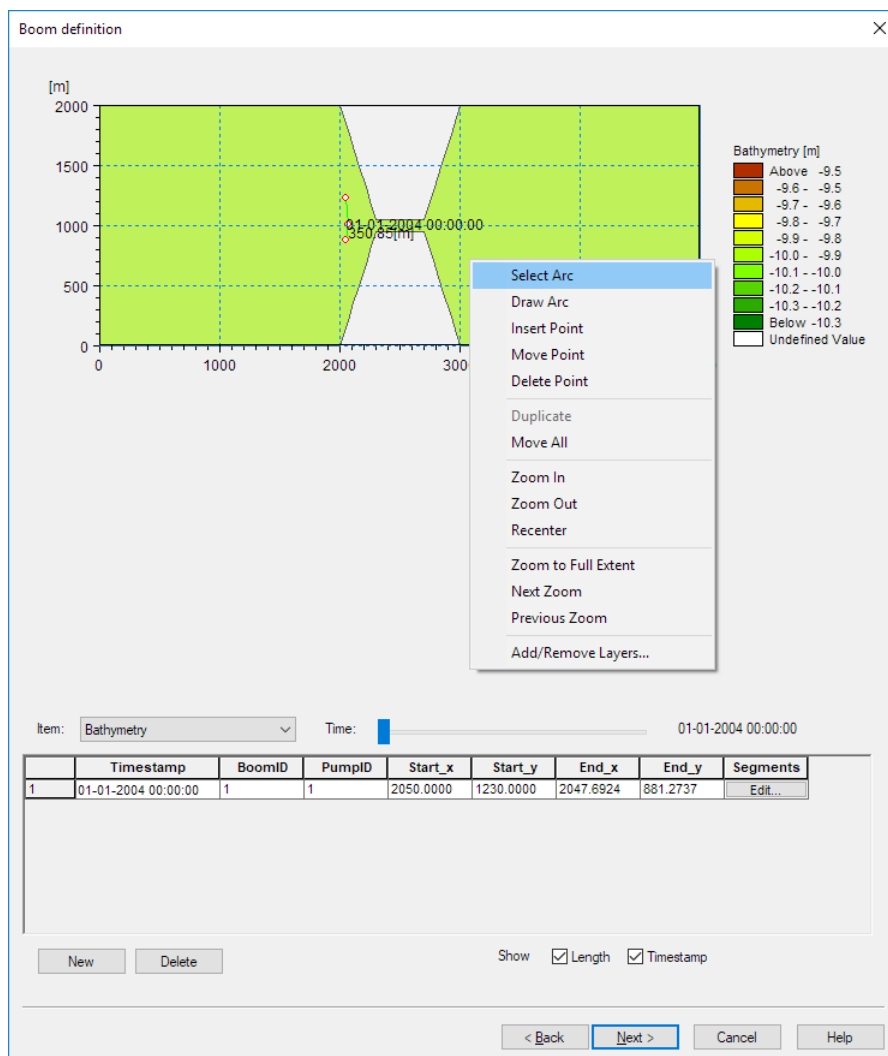
Figure 4.26   Dialog for specifying boom segments in the domain

To insert a new boom segment at the active time step, use the "New" button. This will add a boom to the definition table and set it as active boom. The table will just show the start and end point of a boom. To modify individual points of the boom, use the "Edit" button. This will bring up an extra dialogue to modify the individual segments of the boom. You can also use the right-click context menu in the graphic representation to modify the active boom (i.e. add/move/delete nodes, duplicate etc.). The context menu allows also to add a particle track overlay for placing a boom in a oil spill response planning. The time slider can be used to set the active time; note the display shows all time steps and a time stamp is placed next to the start node of each definition.

When creating the boom definition file, the node positions will be interpolated if there are more than one timestamps defined, i.e. one need just to add key frame positions. Pay attention to the fact that the boom will be removed after the last timestamp. If just one timestamp is defined the boom will persist throughout the whole simulation.

When finished with the boom specification the output file has to be defined.
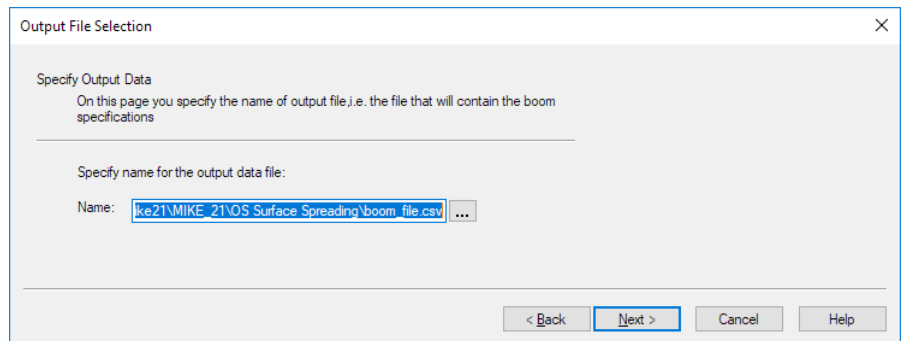
Figure 4.27   Dialog for specifying output file

It is best to place this file with the default name "boom_file.csv" in the simulation root folder. Please note that file name and location used by the oil spill simulation is mandatory. If the result file is named different or placed in a different location it must be manually copied and/or renamed before it is used.

The following status page (Figure 4.28) gives a short overview on the defined booms and allows the user to generate the output file by pressing the "Execute" button. The same will happen if the tool definition is selected and "run" is pressed in the overview.
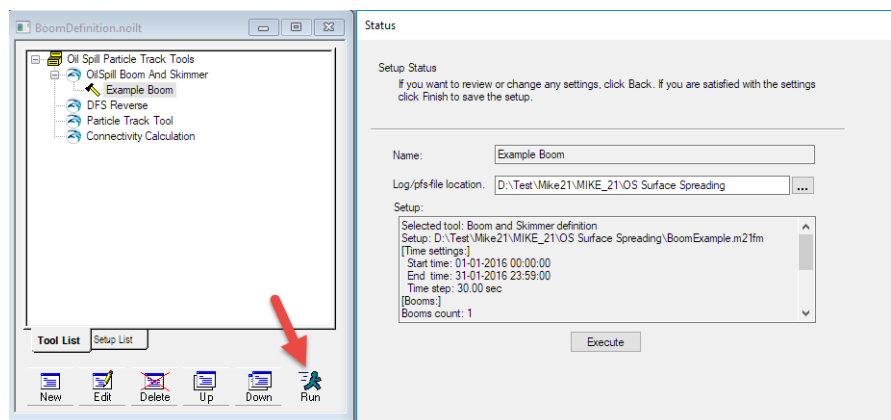
Figure 4.28   'Run' command or Execute from Status page in simulation setup editor

Once the boom definition file has been generated the main simulation can be run.

4.3.4   Results

There is currently no direct way to use the boom definition file to visualise the results. If you want to visualise a boom you can make use of a XYZ-file or dfs1 format.

These file types can then be used in the Data Manager or Result Viewer to visualise a boom. For some technical reasons the Result Viewer is more suited as it can connect the boom nodes. The XYZ format is suitable for stationary booms whereas the dfs1 format can be used for moving booms as well.

To visualise the stationary example boom the node coordinates have to be saved in a XYZ file. This is a plain text file with 4 whitespace separated values representing the x,y,z -coordinates and a connectivity number. An example XYZ file with the coordinates of the boom this looks like:

```
2050.00     1230.00      0.00         1
2067.02     1006.9       0.00         1
2047.69     881.274      0.00         0
```

To be able to visualise the boom the connectivity (4th value) must be specified such that the value in the boom end point in the last line is zero and the other lines have "1".

The file can be added to a Result Viewer view similar as a standard dfsu and the particle file. To draw a line between the points you need to enable it on the line style properties page of the XYZ data.
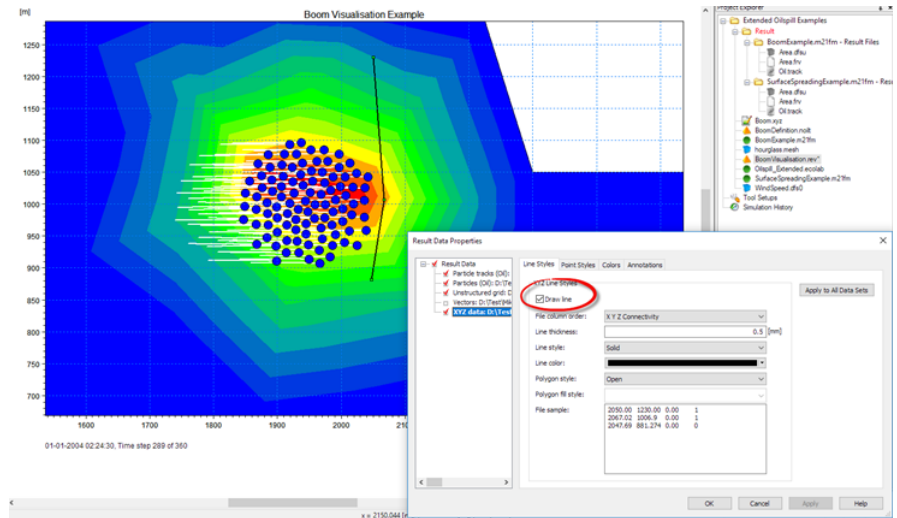
Figure 4.29   Specifying line display based on boom coordinates from xyz data

In the example the flag "Set to one to lock a particle at a boom" is used to colour the particles representing a particles state of being lock at a boom or freely moving on the surface.

The screen dumps in the following figures shows basically the same data as for the surface spreading example. However, a boom is present that block the entrance to the channel connecting the two basins. The oil particles are driven by westerly winds towards the barrier.
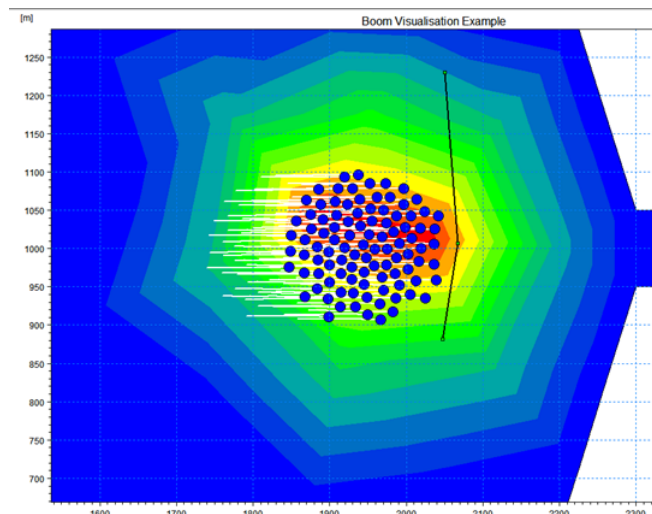
Figure 4.30   Particles before reaching boom

For the time step shown in Figure 4.30 no particles are blocked by the boom yet (compare to the image shown in Figure 4.17). The following figures show

the oil plume just few time steps later and at the end of the simulation. Here a large number of particles are become blocked by the boom (indicated by the red colour).
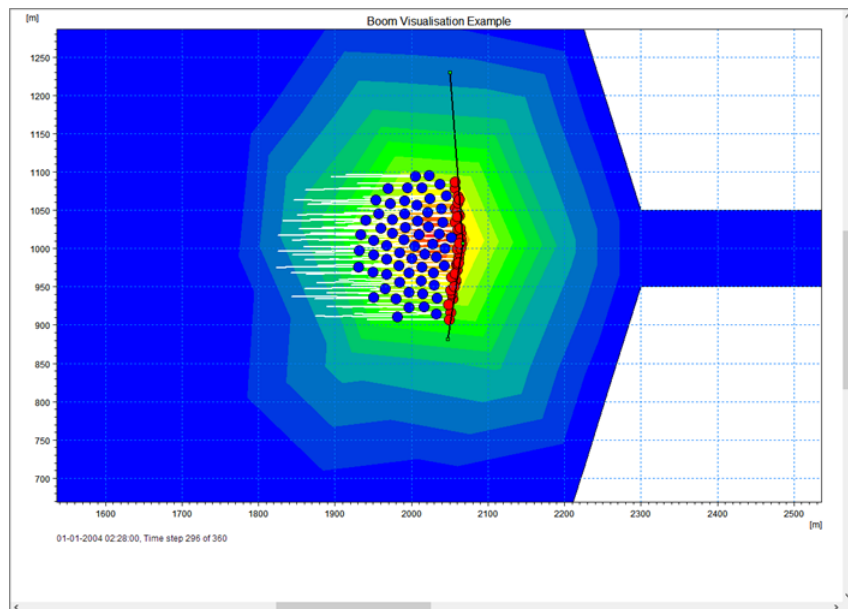
Figure 4.31   Particles when first reaching the boom
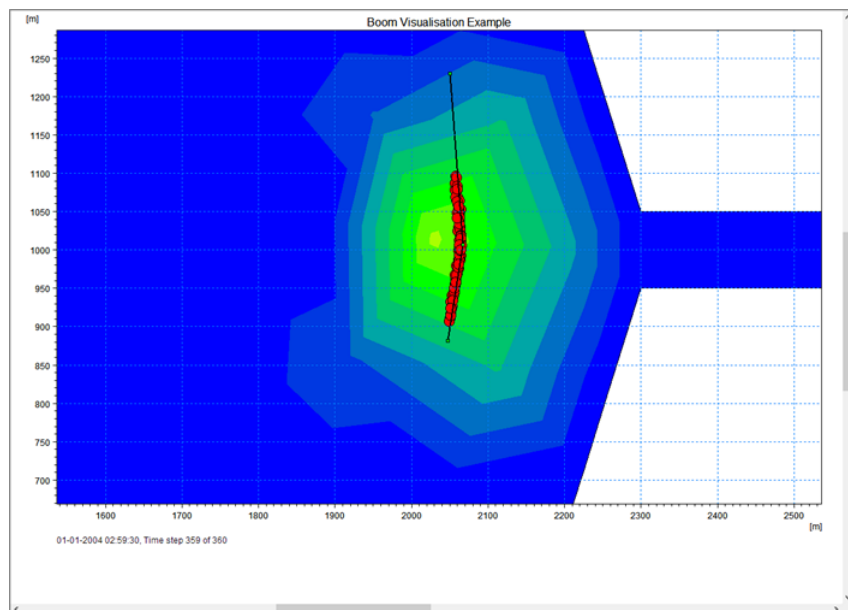
Figure 4.32   Particles at the end of the simulation

Note: the XYZ file can just be used to visualise stationary booms. If booms move in time and space the coordinates can be provided as dfs1 file and plotted similar. Here you need to provide a dfs1 file containing at least 2 items of the type "Geographical coordinate" representing the x/y coordinates of the boom nodes. Add as many grid points as boom nodes. You can just provide keyframe coordinates, i.e. there will be linear interpolation between coordinates in time. When visualising the dfs1 in the Result Viewer select "Type=Spatial line" and "Location=Geographical position" as well as the proper X and Y items in the spatial line properties.

4.3.5   Files

The following data files (included in the \ELOS\Extended_OS folder) are supplied with MIKE 21 Flow Model ELOS FM:

Filename: hourglass.mesh
Description: Mesh file including the mesh and bathymetry

Filename: Oilspill_Extended.ecolab
Description: copy of extended oilspill template (ECO Lab Template)

Filename: BoomExample.m21fm
Description: MIKE 21 Flow Model FM specification file

Filename: WindSpeed.dfs0
Description: Wind data used in simulation

Filename: BoomDefinition.noilt
Description: Oil Spill Particle Track toolbox file containing an oil spill boom and skimmer definition to generate the boom data file

Filename: boom_file.csv
Description: Boom data file generated by the oil spill boom and skimmer definition

Filename: Boom.xyz
Description: manually created XYZ file containing the stationary boom nodes for visualisation purpose only.

Filename: BoomLine.dfs1
Description: manually created dfs1 file containing a moving boom for visualisation purpose only.

Filename: BoomVisualisation.rev
Description: Result viewer setup for the simulation results, showing the simulation area, oil particles and the stationary boom using a XYZ-file.

Filename: BoomVisualisation_lines.rev
Description: Result viewer setup for the simulation results, showing the simulation area, oil particles and a moving boom using a dfs1-file.

5 MIKE ECO LAB / OIL SPILL MODULE

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 using process oriented formulations.

Besides the pure process orientated description MIKE ECO Lab also supports the characterisation of individual spatial entities (or particles) with associated attributes, processes and description of their movement. Such entities can represent different individuals like fish or particles like oil parcels.

5.1 Model Definition

In this dialog you specify a MIKE ECO Lab template, representing the actual model formulation and the solution parameters: Integrated Method and Update Frequency.

5.1.1 Template selection

A MIKE ECO Lab template contains mathematical equations describing an aquatic ecosystem. The user has two options:

- Using one of the DHI supported predefined MIKE ECO Lab templates or the DHI supported predefined oil spill templates
(Note: the predefined oil spill templates must be imported using 'From file...', and can be found in the installation folder under .\MIKE Zero\2023\Templates\OS)

- Using another MIKE ECO Lab template or oil spill template. Choose 'From file...'

Having selected the 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 3 ECO Lab / Oil Spill dialogs are reset to default values. Especially the user parameterisation of constants and forcing is reset to the default values stored in the template. However, the MIKE ECO Lab Parameter set library provides an easy mechanism to store and retrieve a complete parameterisation and makes reloading/updating of a template simple.

Predefined MIKE ECO Lab templates

The installation contains a number of standard MIKE ECO Lab templates. They can be used for a variety of process oriented investigations as well as investigations concerning the behaviour of individual entities.

You can find a description of the available templates in the MIKE Zero Documentation Index that can be accessed from the start menu. This is also where you can find a description of the available Oil Spill templates.

Load Parameter set

You can load a set of previous specified parameters, i.e. populate the MIKE ECO Lab constants and forcing settings with previous specified values. You can also invoke the MIKE ECO Lab Parameter set library by pressing the library button. After applying a parameter set a short summary will be shown, listing the successful matched parameters and occurred errors/warnings. Please note that the matching algorithm operates on the MIKE ECO Lab symbol names and element types, i.e. it is possible that a collection and the setup contain different numbers of specified parameters or may be based on different MIKE ECO Lab templates (versions). If parameters refer to data files the user must play attention to make these data files available.

5.1.2   MIKE ECO Lab Parameter set library

The MIKE ECO Lab parameter set library can be used to maintain different parameterisations, i.e. value settings for the MIKE ECO Lab constants and forcing. A single parameterisation, i.e. the specific value settings for all the (Eulerian and ABM) MIKE ECO Lab constants and forcing is called a parameter set. Such sets can be stored (and retrieved) from individual files, so called parameter set collections. The parameter set library consist of at least one or more such collections.

The default collection is the startup collection and represents the parameterisation of the initially loaded setup. It is neither possible to add nor to remove this default collection or to add/delete sets to it. The main purpose of the startup collection is be able to revert to the initial states stored in the setup (it does not necessarily reflect the defaults/initial value settings of the template). To add a new, user defined collection use the "new" button and specify the storage location and file name in the following dialogue. Please note that existing files will be overwritten without further notice! The "load" button can be used to open an existing parameter collection file, i.e. make all stored settings available in the load parameter list (see Template selection). 'The "unload" button will remove the access to selected collection and all its sets but will not delete the collection file.

To add the current active value specifications of the MIKE ECO Lab setup, i.e. the constants and forcing specification, to a collection, select the collection and press the "add" button. This will append the collection and add a new parameter set. You can specify a name and a short description text for both the collection and for each stored parameter set that will be used to identify a specific set. To update an existing parameter set with the current value settings, select the set and use the "update" button. This will overwrite the stored specifications with the current values from the setup.

To leave the parameter set library use the "close" or "save and close" buttons. The later will write any new/updated set (marked with a "*" in front of their name) to the specified collection files.

5.1.3 Integration method

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 (not available in ABM Lab)

Euler integration method

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

The formula for the Euler method is:

$$y_{n+1} = y_n + h \cdot f(x_n, y_n) \tag{5.1}$$

which advances a solution y from x_n to $x_n+1 = x_n + h$

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.

$$y_{n+1} = \mathrm{rk4}(y_n, f(x_n, y_n), x_n, h) \tag{5.2}$$

The function is solved this way:

$$k_1 = h \cdot f(x_n, y_n) \tag{5.3}$$

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

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

$$k_4 = h \cdot f(x_n + h, y_n + k_3)$$

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

which advances a solution y from x_n to $x_n + 1 = x_n + h$

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.

$$y_{n+1} = f(y_n, f(y_n, x_n), \ x_n, h, \varepsilon, \text{yscale}) \tag{5.4}$$

The function is solved this way:

First take two half steps:

$$h_2 = 0.5 \cdot h \tag{5.5}$$

$$x_{n+\frac{1}{2}} = x_n + h_2 \tag{5.6}$$

$$y_2 = \text{rk4}(y_n, f(y_n, x_n), \ x_n, h_2) \tag{5.7}$$

$$y_2 = \text{rk4}(y_2, f(y_2, x_{n+\frac{1}{2}}), \ x_{n+\frac{1}{2}}, h_2) \tag{5.8}$$

Compare with one full time step:

$$y_1 = \text{rk4}(y_n, f(y_n, x_n), \ x_n, h) \tag{5.9}$$

Then estimate error:

$$y_1 = y_2 - y_1 \qquad (5.10)$$

$$\text{err} = \text{MAX}(\text{ABS}(y_1/\text{yscale}))/\varepsilon \qquad (5.11)$$

If the error is small (err <= 1.0) the function returns

$$y_{n+1} = y_2 + \frac{y_1}{15} \qquad (5.12)$$

which advances a solution y from x_n to $x_n + 1 = x_n + h$

or else the time step is reduced and the function tries again.

5.1.4 Update frequency

The time step for the update of the MIKE ECO Lab equations is the overall time step (specified on the Time dialog) multiplied by the Update Frequency.

Selecting 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.

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

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 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.

Be aware that the following also influence CPU time:

- the choice of MIKE ECO Lab integration method
- the number and complexity of the mathematical expressions in the MIKE ECO Lab template
- the MIKE ECO Lab update frequency

5.1.5 Options

Compute in dry elements

If this option is enabled, ECO Lab is run on all elements, regardless of their flood/dry status. For performance, ECO Lab calculations are usually just performed on "real wet" elements, similar to AD transport calculations, i.e. dry elements are skipped. Enabling the calculation on dry elements will allow you to calculate fixed (not transported) ECO Lab items, i.e. fixed state variables. The concentrations of any transported state variable/ AD component will be set to zero in all elements considered dry and not be updated. Enabling the dry element calculation will also cause the output of all fixed state variables in dry elements. Please note that process/auxiliary variables are not written by default in dry elements. If you need these, ensure that the output specification uses the flood and dry type "whole area".

Optimise unused equations

Enabling this option may speed up the calculation time of ECO Lab. Before the simulation start, the ECO Lab core will replace any calculation expression of unused variables with a constant value, i.e. it will not waist time in calculating unnecessary expressions. "Unused" in this context means that the expression is not direct or indirect relevant as a model result output and it has no side effects[1]. Please note that the runtime becomes dependent on the output specifications.

Disable Process

This is an option considered relevant only during model development/setup. It allows to fully skip all ECO Lab calculations, i.e. just the necessary AD transport and utility calculations are performed. If enabled, the model results correspond to a setup with the corresponding number of AD components.

5.2 Classes

The Classes dialog shows a summary of the classes defined in the selected model definition. This dialog is only visible if the chosen template contains a valid particle class description.

---

1 Side effects are indirect effects on the calculations. For example, the computation of random numbers has some side effects. Skipping/removing one random number calculation would change the sequence of numbers created by the pseudo-random generator and potentially cause a different simulation outcome. Similar, skipping a call to an external plugin could result in unintended behavior. Therefore, expressions with these and a number of other functions are not replaced/ optimised.

The name and description of each class variable are given. From the list view you can go to the dialog for specification by clicking on the "Go to.." button.

5.2.1 General description

Each particle class may be defined by a number of attributes like state variables, constants and restricted area search functions. State variables of a class represent internal states and they are the variables the user wants usually to predict. Constants usually represent rates or thresholds whereas restricted area search functions are used by a particle to interact/sense the environment.

5.2.2 Class specification

This single class overview page is just a static information page listing the class name and description and the number of pre-defined state variables, constants, arithmetical and restricted area search functions of this specific class.

State variables

The state variables dialog shows a summary of the state variables defined. The state variables are static.

Constants

The class constants dialog lists all constants defined for this class with their name, description and unit together with a user-defined numeric value. The number and type of constants cannot be modified. If no class constants are defined the dialog is not shown.

Restricted area search functions

The class restricted area search functions page lists all restricted area search functions defined for this class with their number and description. The number and type of functions cannot be modified. If no spatial constants are defined the dialog is not shown.

5.3 State Variables

The state variables dialog 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. If no state variables are defined the dialog is not shown.

5.3.1   General description

State variables are usually the most important variables in a process oriented 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 set-up. The state variable will change according to how the processes that the model developer describes affects 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.

5.3.2   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.

5.3.3   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/m^2]. 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.

5.4   Solution Technique

The simulation time and accuracy can be controlled by specifying the order of the numerical schemes which are used in the numerical calculations. Both the scheme for time integration and for space discretization can be specified. You can select either a lower order scheme (first order) or a higher order scheme. The lower order scheme is faster, but less accurate. For more details on the numerical solution techniques, see the scientific documentation. If no state variables are defined this dialog is not shown.

The time integration of the shallow water equations and the transport (advection-dispersion) equations is performed using a semi-implicit scheme, where the horizontal terms are treated explicitly and the vertical terms are treated implicitly. Due to the stability restriction using an explicit scheme the time step interval must be selected so that the CFL number is less than 1. A variable time step interval is used in the calculation and it is determined so that the CFL number is less than a critical CFL number in all computational nodes. To control the time step it is also possible for the user to specify a minimum time step and a maximum time step. The time step interval for the transport equations is synchronized to match the overall time step specified on the Time dialog.

The minimum and maximum time step interval and the critical CFL number is specified in the Solution Technique dialog in the HYDRODYNAMIC MODULE.

5.4.1   Remarks and hints

If the important processes are dominated by convection (flow), then higher order space discretization should be chosen. If they are dominated by diffusion, the lower order space discretization can be sufficiently accurate. In general, the time integration method and space discretization method should be chosen alike.

Choosing the higher order scheme for time integration will increase the computing time by a factor of 2 compared to the lower order scheme. Choosing the higher order scheme for space discretization will increase the computing time by a factor of 1½ to 2. Choosing both as higher order will increase the computing time by a factor of 3-4. However, the higher order scheme will in general produce results that are significantly more accurate than the lower order scheme.

The default value for the critical CFL number is 1, which should secure stability. However, the calculation of the CFL number is only an estimate. Hence, stability problems can occur using this value. In these cases you can reduce the critical CFL number. It must be in the range from 0 to 1. Alternatively, you can reduce the maximum time step interval. Note, that setting the minimum and maximum time step interval equal to the overall time step interval specified on the Time dialog, the time integration will be performed with constant

time step. In this case the time step interval should be selected so the the CFL number is smaller than 1.

The total number of time steps in the calculation and the maximum and minimum time interval during the calculation are printed in the log-file for the simulation. The CFL number can be saved in an output file.

The higher order scheme can exhibit under and over shoots in regions with steep gradients. Hence, when the higher order scheme is used in combination with a limitation on the minimum and maximum value of the concentration, then mass conservation cannot be guarenteed.

5.5 Constants

In the MIKE ECO Lab Constants dialog the MIKE ECO Lab constants defined in the MIKE ECO Lab template can be modified. If no constants are defined the dialog is not shown.

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
- 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 template, it can be specified as a "Constant value", a "Type 2 data file" or a dfsu file with one time step.

NOTE: A constant, which is defined as a built-in constant in the MIKE ECO Lab template, will appear as a user-defined constant in case it is not supported by MIKE 3 Flow Model FM.

5.5.1 General description

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.

5.5.2 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 in MIKE 3 Flow Model FM:

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 duration of time 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.

5.5.3 Remarks and hints

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.

5.6 Forcings

In the MIKE ECO Lab Forcings dialog 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
- 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", a "Type 2 data file" or a dfsu file. The data files have to cover the entire simulation period. In case a type 2 file is allowed for, it must cover the spatial extent and coordinates of the mesh file.

NOTE: 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 3 Flow Model FM.

5.6.1 General description

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.

5.6.2 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 one layered grid systems the water depth will be returned

2. Salinity. If available, this forcing returns the salinity calculated in the hydrodynamic set-up

3. Temperature. If available, this forcing returns the temperature calculated in the hydrodynamic set-up

4. Wind velocity. If available, this forcing returns the wind velocity specified in the hydrodynamic set-up

5. Wind direction. If available, this forcing returns the wind direction specified in the hydrodynamic set-up

6. Water surface level. This forcing returns the water level calculated in the hydrodynamic set-up

7. Water depth. This forcing returns the water depth calculated in the hydrodynamic set-up

8. Horizontal current speed. This forcing returns the horizontal current speed calculated in the hydrodynamic set-up

9. Horizontal current direction. This forcing returns the horizontal current direction calculated in the hydrodynamic set-up

10. Vertical current speed. This forcing returns the vertical current speed calculated in the hydrodynamic set-up

11. Water surface slope in flow direction. This forcing returns the slope of the water surface calculated in the hydrodynamic set-up. Under normal conditions positive values.

12. Water density. If available in hydrodynamic simulation this forcing returns a value for water density

5.6.3 Remarks and hints

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.

5.7 Dispersion

In numerical models the dispersion usually describes transport due to non-resolved processes. In coastal areas it can be transport due to non-resolved turbulence or eddies. Especially in the horizontal directions the effects of non-resolved processes can be significant, in which case the dispersion coefficient formally should depend on the resolution.

In a 3D model it is important to distinguish between horizontal dispersion due to e.g. non-resolved eddies, and vertical dispersion due to e.g. bed generated turbulence. Hence, dispersion in horizontal and vertical directions is specified separately.

The dispersion is specified individually for each AD state variable and for each particle class.

5.7.1 Dispersion specification

The dispersion can be formulated in one of three ways

- No dispersion
- Dispersion coefficient formulation
- Scaled eddy viscosity formulation

Selecting the dispersion coefficient formulation you must specify the dispersion coefficient.

Using the scaled eddy viscosity formulation the dispersion coefficient is calculated as the eddy viscosity used in solution of the flow equations multiplied by at scaling factor. For specification of the eddy viscosity see section 6.6, Eddy Viscosity.

Data

Selecting dispersion coefficient option the format of the dispersion coefficient can be specified as

- Constant (in both time and domain)
- Varying in domain

For the case with dispersion coefficient varying in domain the values are constant in the vertical domain and only varying in the horizontal domain. You have to prepare a data file containing the dispersion coefficient before you set up the hydrodynamic simulation. The file must be a 2D unstructured data file (dfsu) or a 2D grid data file (dfs2). The area in the data file must cover the model area. If a dfsu-file is used, a piecewise constant interpolation is used to map the data. If a dfs2-file is used, a bilinear interpolation is used to map the data.

Selecting Scaled eddy viscosity option the format of the scaling factor can be specified as

- Constant
- Varying in domain

For the case with values varying in domain you have to prepare a data file containing the scaling factor before you set up the hydrodynamic simulation. The file must be a 3D unstructured data file (dfsu) or a 3D data grid file (dfs3). The area in the data file must cover the model area. If a dfsu-file is used, a piecewise constant interpolation is used to map the data. If a dfs3-file is used, a bilinear interpolation is used to map the data.

5.7.2   Recommended values

When more sophisticated eddy viscosity models are used, as the Smagorinsky or k-ε models, the scaled eddy formulation should be used.

The scaling factor can be estimated by $1/\sigma_T$, where σ_T is the Prandtl number. To be consistent with the empirical constants for the k-ε turbulence model the value of σ_T should be the same as the value for the Prandtl number specified on the Equation dialog in the TURBULENCE MODULE. The default value here for the Prandtl number is 0.9 corresponding to a scaling factor of 1.1.

The dispersion coefficient is usually one of the key calibration parameters for the Transport Module. It is therefore difficult to device generally applicable values for the dispersion coefficient. However, using Reynolds analogy, the dispersion coefficient can be written as the product of a length scale and a velocity scale. In shallow waters the length scale can often be taken as the water depth, while the velocity scale can be given as a typical current speed.

Values in the order of 1 are usually recommended for the scaling factor for the horizontal plane. For more information see e.g. (Rodi, 1980 /2/).

The scaling factor for the vertical plane is usually much smaller, e.g. 0.00001. As it is a calibration factor this can sometimes even be 0.

5.8 Drift profile

This section is only relevant when including particle classes.

5.8.1 General description

The drift profile is a description of the drift regime that the particles are influenced by. It will normally be the currents and the wind that governs the drift regime. The currents including wind are already calculated in the hydrodynamic setup, but the hydrodynamic output does normally not have a fine discretization of the current profile near the bed. For MIKE 21 FM for instance it is depth average values that are the output of the hydrodynamic setup, and even for MIKE 3 FM the drift conditions near the bed are normally not resolved adequately for describing sediment particles. Therefore it can be a good idea to assume some shapes of the vertical drift profile.

It is possible to include the bed friction drag on the current profile by assuming a bed shear profile (or logarithmic profile). In MIKE 3 FM the bed shear profile is only applied in the bottom layer of the model, and the calculated flow conditions in the other layers are not modified.

The wind drag can also cause increased flow velocities in the upper part of the water column, and corresponding velocities in the opposite direction in the lower part. In MIKE 3 FM this effect can be included in the hydrodynamic output.

If particles are in the water surface, they can be influenced directly by the wind additionally to the influence from the flow. This will result in an additional acceleration of the particle in a direction relative to the wind turned with a wind drift angle caused by coriolis forces.

5.8.2 Class drift profile

The different drift profile types can be combined in the following ways

- Use raw data from hydrodynamics
- Use bed shear profile
- Use surface wind acceleration
- Use bed shear profile and surface wind acceleration

Depending on the choice of drift profile you specify some additional parameters.

Bed shear profile

The shape of the velocity profile within a turbulent boundary layer is well established by both theory and experience. The profile has specific charac-

teristics very close to the bed where viscosity controls the vertical transport of momentum, and different characteristics farther from the bed where turbulence controls the vertical transport of momentum. The region closest to the bed boundary is called the laminar sub-layer or viscous sub-layer, because within the region turbulence is suppressed by viscosity. The laminar sublayer only plays a significant role for smooth flows, whereas for rough flows the flow is zero for z smaller than z_0.

Logarithmic layer (z >= δ_s smooth flow) (z >= z_0 rough flow)

$$u = \frac{2,3}{k} \cdot u^* \cdot \log_{10}\frac{x}{z_o} \qquad (5.13)$$

where

u^*:	Friction velocity
k:	Karman constant = 0.4
z_0:	characteristic roughness

Surface wind acceleration

The user must specify wind weight, wind drift angle and the kinematic viscosity in order to calculate the surface wind acceleration.

Particles that are exposed to wind in the water surface are affected according to the wind regime in 2 ways: Indirectly via the currents that include the wind, but also directly as an extra force on the particle. How much of the wind speed that are transferred to the particle speed depends on the nature of the particle, how much is the particle exposed etc, so therefore it is a calibration factor that expresses how much of the windspeed that is added to the particle speed.

$$
\begin{aligned}
U_{particle} &= U_{current} + C_w \cdot W \cdot \sin(\theta_{dir} - \pi + \theta_w) \\
V_{particle} &= V_{current} + C_w \cdot W \cdot \cos(\theta_{dir} - \pi + \theta_w)
\end{aligned}
\qquad (5.14)
$$

where

C_w:	Calibration factor for wind drag on particle
θ_{dir}:	Wind direction
θ_w:	Wind drift angle

Wind drift angle

The coriolis force is normally included in the hydrodynamic currents, but for the wind acceleration of surface particles the coriolis force must be considered as well.

Due to the influence from the Coriolis force, the direction of the wind drift vector is turned relatively to the wind direction. The angle *qw* of deviation is

termed with the wind drift angle. It turns to the right on the Northern Hemisphere and to the left on the Southern Hemisphere. Thus wind drift angles for the Southern Hemisphere should be specified by negative values. From Al-Rabeh (1994), it is assumed that

$$\theta_w = \beta \exp\left(\frac{\alpha |U_w|^3}{g\gamma_w}\right)$$

(5.15)

where

α:	$-0.3 \cdot 10^{-8}$
β:	$28° \, 38'$
γ_w:	Kinematic viscosity [m^2/s]
g:	Gravity [m/s^2]

The magnitude of the wind drift angle varies with the geographical location and wind speed and it is often estimated at 12-15 degrees in the North Sea.

Wind induced profile

Wind induced profile can only be applied for 2D simulations.

5.9 Bed Roughness

This section is only relevant when including particle classes.

The bed roughness is used in the particle transport sub-model if the class drift profile is defined as a bed shear profile (logarithmic profile). It is an important parameter for describing the near bed flow conditions.

The bed roughness can be specified as

- Bed roughness from hydrodynamic model
- User specified bed roughness

5.9.1 General description

The bed roughness in the particle transport sub-model is defined by the Nikuradse roughness *ks*. This roughness parameter may be converted from other roughness definitions as described below.

Chezy number conversion to Nikuradse roughness *ks*:

$$k_s = \frac{12h}{10^{(C/18)}}$$

(5.16)

where

h: Water depth
C: Chezy number

Manning number conversion to Nikuradse roughness ks:

$$k_s = \left(\frac{25,4}{M}\right)^6 \tag{5.17}$$

where M is the Manning number.

The quadratic drag coefficient can not be converted automatically.

5.9.2 Bed roughness from hydrodynamic model

The bed resistance is often already specified in the hydrodynamic setup.

In MIKE 3 FM bed resistance can have been specified as Quadratic drag coefficient, or roughness height.

The quadratic drag coefficient can not be converted automatically, and instead the user must specify Nikuradse roughness directly. If the bed resistance in the hydrodynamic module is specified as roughness height, no conversion is needed.

5.9.3 User specified bed roughness

The bed roughness must be specified as Nikuradse roughness and it can be specified as

- Constant
- Varying in domain

For the case with values varying in domain you have to prepare a data file containing the bed roughness before you set up the hydrodynamic simulation. The file must be a 2D unstructured data file (dfsu) or a 2D grid data file (dfs2). The area in the data file must cover the model area. If a dfsu-file is used, a piecewice constant interpolation is used to map the data. If a dfs2-file is used, a bilinear interpolation is used to map the data.

5.10 Wind Forcing

This section is only relevant when including particle classes.

The wind forcing is used in the particle transport sub-model if the Class drift profile is defined using the influence from wind.

The wind forcing can be specified as

- User specified wind, speed and direction
- User specified wind and velocity components
- Wind from hydrodynamic model

5.10.1 User specified wind

The wind forcing can be specified as

- Constant
- Varying in time, constant in domain
- Varying in time and domain

For the case with values varying in domain you have to prepare a data file containing the wind forcing (speed and direction (in degrees from true North) or velocity components) before you set up the hydrodynamic simulation. The file must be a 2D unstructured data file (dfsu) or a 2D grid data file (dfs2). The area in the data file must cover the model area. If a dfsu-file is used, a piece-wice constant interpolation is used to map the data. If a dfs2-file is used, a bilinear interpolation is used to map the data.

Furthermore a soft start interval must be specified.

5.11 Precipitation-Evaporation

If your simulation includes precipitation and/or evaporation, you need to specify the concentration of each AD state variable in the precipitated and evaporated water mass. The precipitation and evaporation can be included in two ways

- Ambient concentration.
  The concentration of the precipitated/evaporated water mass is set equal to the concentration of the ambient sea water.
- Specified concentration.
  The concentration of the precipitated/evaporated water mass is specified explictly.

If you have chosen the net precipitation option in the Precipitation-Evaporation dialog in the HYDRODYNAMIC MODULE, the precipitation concentration will be used when the specified net-precipation is positive. When the net-precipitation is negative, the evaporation concentration is used.

The precipitation-evaporation is specified individually for each AD state variable.

5.11.1   Specification

Data

Selecting the specified concentration option the format of the concentration (in component unit) can be specified as

- Constant (in both time and domain)

- Varrying in time and constant in domain

- Varying in both time and domain

For the case with concentration varying in time but constant in domain you have to prepare a data file containing the concentration (in component unit) before you set up the hydrodynamic simulation. The data file must be a time series file (dfs0). The data must cover the complete simulation period. The time step of the input data file does not, however, have to be the same as the time step of the hydrodynamic simulation. A linear interpolation will be applied if the time steps differ.

For the case with concentration varying both in time and domain you have to prepare a data file containing the concentration (in component units) before you set up the hydrodynamic simulation. The file must be a 2D unstructured data file (dfsu) or a 2D grid data file (dfs2). The area in the data file must cover the model area. If a dfsu-file is used, a piecewice constant interpolation is used to map the data. If a dfs2-file is used, a bilinear interpolation is used to map the data. The data must cover the complete simulation period. The time step of the input data file does not, however, have to be the same as the time step of the hydrodynamic simulation. A linear interpolation will be applied if the time steps differ.

Soft start interval

You can specify a soft start interval during which the precipitation/evaporation concentration is increased linearly from 0 to the specified values of the precipitation/evaporation concentration. By default the soft start interval is zero (no soft start).

5.11.2   Recommended values

Usually it is most sensible to set the concentration of the evaporated water mass to zero, in which case the component is conserved in the water.

5.12   Infiltration

If your simulation includes infiltration you need to specify the concentration of each AD state variable in the infiltrated water mass. This can be done two ways

- Ambient concentration.
  The concentration in the infiltrated water mass is set equal to the concentration in the ambient sea water.

- Specified concentration.
  The concentration in the infiltrated water mass is specified explictly.

Data

Selecting the specified concentration option the format of the concentration can be specified as:

- Constant (in both time and domain)
- Varying in time and constant in domain
- Varying in time and domain

For the case with concentration varying in time but constant in domain you have to prepare a data file containing the concentration (in component unit) before you set up the hydrodynamic simulation. The data file must be a time series file (dfs0). The data must cover the complete simulation period. The time step of the input data file does not, however, have to be the same as the time step of the hydrodynamic simulation. A linear interpolation will be applied if the time steps differ.

For the case with concentration varying both in time and domain you have to prepare a data file containing the concentration (in component units) before you set up the hydrodynamic simulation. The file must be a 2D unstructured data file (dfsu) or a 2D grid data file (dfs2). The area in the data file must cover the model area. If a dfsu-file is used piecewice constant interpolation is used to map the data. If a dfs2-file is used bilinear interpolation is used to map the data. The data must cover the complete simulation period. The time step of the input data file does not, however, have to be the same as the time step of the hydrodynamic simulation. A linear interpolation will be applied if the time steps differ.

Soft start interval

You can specify a soft start interval during which the infiltrated concentration is increased linearly from 0 to the specified values of the infiltrated concentration. By default the soft start interval is zero (no soft start).

5.13   Sources

Point sources of dissolved components are important in many applications as e.g. release of nutrients from rivers, intakes and outlets from cooling water or desalination plants.

In the MIKE ECO Lab Module, the source concentrations of each component in every sources point can be specified. The number of sources, their generic

names, location and discharges magnitude are specified in the Sources dialog in the HYDRODYNAMIC MODULE.

Depending on the choice of property page you can see a geographic view or a list view of the sources.

The source concentrations are specified individually for each source and each component. From the list view you can go to the dialog for specification by clicking on the "Go to.." button.

5.13.1 Source specification

The type of sources can be specified in two ways

- Specified concentration
- Excess concentration

The source flux is calculated as $Q_{source} \cdot C_{source}$ where Q_{source} is the magnitude of the source and C_{source} is the concentration of the source. The magnitude of the source is specified in the Sources dialog in the HYDRODYNAMIC MODULE.

When selecting the specified concentration option the source concentration is the specified concentration if the magnitude of the source is positive (water is discharged into the ambient water). The source concentration is the concentration at the source point if the magnitude of the source is negative (water is discharge out the ambient water). This option is pertinent to e.g. river outlets or other sources where the concentration is independent of the surrounding water.

When selecting the excess concentration option the source concentration is the sum of the specified excess concentration and concentration at a point in the model if the magnitude of the source is positive (water is discharge into the ambient water). If it is an isolated source the point is the location of the source. If it is a connected source, the point is the location where water is discharged out of the water. The source concentration is the component concentration at the source point if the magnitude of the source is negative (water is discharged out of the ambient water).

Data

The format of the source information can be specified as

- Constant (in time)
- Varying in time

For the case with source concentration varying in time you have to prepare a data file containing the concentration (in concentration units) of the source before you set up the hydrodynamic simulation. The data file must be a time

series file (dfs0). The data must cover the complete simulation period. The time step of the input data file does not, however, have to be the same as the time step of the hydrodynamic simulation. A linear interpolation will be applied if the time steps differ.

5.13.2 Remarks and hints

Point sources are entered into elements, such that the inflowing mass of the component initially is distributed over the element where the source resides. Therefore the concentration seen in the results from the simulation usually is lower than the source concentration.

5.14 Particle Sources

Particle sources are only available when the chosen template defines at least one valid particle class. A particle source is used to introduce members or particles of a specific class into the model. Particle sources do not depend on water inflow and thus must be specified independently of hydraulic sources.

By switching property page you can see a Geographic View or a List View of the sources. New sources can be added to both these views.

In the List View you can create a new source by clicking on the "New source" button. By selecting a source in the Source list and clicking on the "Delete source" you can remove this source. For each source you can specify the name of the source and whether the source should be active or not. The specification of detailed information for each source is made subsequently. From the List View page you can go to the dialog for specification by clicking on the "Go to .." button.

In the Geographic View it is also possible to create a new source by selecting "Add new..." from the context menu. The geographical position of the source is set to the mouse pointer coordinates and depending on the source type, the source location can then be edited by dragging the source symbols on the map. The additional information for the source is made subsequently.

5.14.1 Particle source specification

Three general types of source layouts can be specified:

- Point source
- Area source
- File Source

Each of the source layouts has several sub-types. In general, point sources specify a single, defined point in space whereas area sources describe a spatial domain where particles are released. In case of a file source the release

locations and particle states are read from a file. A normal source is active throughout the complete simulation time. An initial source is used to specify an initial particle distribution and does not release any particles during the rest of simulation.

A source may include one or many different types of particle classes. The additional information for each particle class is made subsequently. You may choose to include or exclude the defined classes in the simulation.

Coordinates

You have to specify the map projection (Longitude/Latitude, UTM, etc.) in which you want to specify the location coordinates of the particle source. In case of a file source the release coordinates are read from a data file.

Vertical source specification

Apart from the horizontal specification, a source location must be specified vertically in the water column. Three definitions are available for the vertical positioning of a source. The vertical reference can be defined as :

- Depth (positive downwards from the moving water surface)

- Above bed (positive upwards relative to the sea bed)

- Datum (absolute level)

An area source may further spawn over a range in the water column. In this case a vertical layer thickness has to be given. The vertical position of a released particle is then randomly selected within the defined layer, i.e. extending from the reference point plus the layer thickness. All data on vertical position refer to the length unit. If the source definition causes a particle to be released above surface/below bed level, the position is set to the surface/bed respectively. In case of a file source the vertical position is read from the data file.

Point source

The location of a point source must be defined using one of two sub-types

- Fixed location
- Moving location

For the fixed location source option , i.e. the source is stationary during simulation time, you must specify the horizontal coordinates of the source point and its vertical position.

For the moving location source option, i.e. the source is moving along a defined path, you must specify a time series file (dfs0) that contains the horizontal coordinates and the vertical position of the source as a function of time. The unit of the vertical position is meters and the value is to be given according to the defined vertical type.

Area source

The location of an area source must be defined using one of two sub-types

- Point collection
- Contour/Shape

An area source describes either a collection of individual (fixed) points or a geometric shape. A point collection can be an irregular placed group of individual points or a regular grid within a defined rectangle. When declaring a contour/shape source particles are released in the space covered by a geometric figure. In all cases the specifications of the released particles is valid for any location within the source.

Particle casting

Particles are placed within the area covered by the area source definition. It may be that the described area includes land elements (e.g. a small island, land borders etc.). In this case a particle potentially can be placed outside the domain. If this happens, the particle may be re-casted to find a valid location in the domain a given number of times. If this finally does not succeed, the particle may be ignored (skip to the next particle) or the simulation will be stopped with an error. Note that the amount of released substances will probably not match your expectations if particles are ignored as the particle associated items will not enter the simulation!

Point collection

Point collections describe a number of individual, fixed source locations in the horizontal plane belonging to the same source. Such a collection is defined by one of two area definitions

- Regular grid
  (points located at the cell centers in a given rectangular grid)
- Irregular point collection
  (irregular placed, individual points)

The advantage over individual fixed point sources is that the item definitions refer all release points.

Particle placing

Depending on the grid type the release locations will be used sequential (row by column, column by row) or randomly permuted. Note that all positions inside a point collection have to be used before a particle can be released at the same position again, e.g. if there are 15 points in total and 15 particle per time step are released, every location will receive one particle. Thus even if random filling is selected all release locations will be used before a new permutation is selected.

Regular grid

In case of a regular grid the anchor point describes the lower left corner of the rectangle covering the source area. The source rectangle extends a given width along the X-axis and a height along the Y-axis and may be rotated around the anchor point. The area is divided into a regular grid of N x M columns and rows. The actual particle release positions are located at the crossing/centres of the columns and rows.

Irregular point collection

An irregular grid consists of a number of individual, irregular placed points in the horizontal plane.

Contour/Shape

A contour/shape source is defined by a set of points in the horizontal plane and a number of elements made of these points to describe the actual release area. Every release element must be characterised by three points. Depending on the selected points the release location will be a single location (all points of the element are the same), a line (2 points are the same) or a triangle (three different points). The final release location is a random point on a line element or inside a triangle element. Both the points and elements have to be created manually and the first point must be placed inside the domain (water point). Subsequent points may be placed outside water elements.

Particle placing

Normally particle placing is based on the total area. In this way particles cover the total source area (covered by all elements) uniformly. Please note that by definition elements describing single locations (all points in the element are the same) or elements describing a line (two points are the same) do not have an area. If particles are placed based on the total area, such elements will not receive any particles! In this case the particles should be placed based on the sub-element count. By doing this, every sub element has the same probability to receive a particle.

Released class items

The number of particles to be released into the flow per overall time step can be a constant number (same number every time step) or the number of released particles can be read from a time series data file (dfs0). Be aware that interpolation between data points may lead to an unexpected number of particles, thus it is best to provide a data series with the same time resolution than the simulation.

The individual state variables/class items can be specified separately. In general the release format for a state variable can be constant, time varying or from a specified distribution. The source data will be checked against the allowed minimum/maximum item value. If the source value is outside this range, the value will be clipped to ensure that the item value will not violate the minimum/ maximum.

Certain state variables, e.g. a length or a gender indicator, etc., have to be declared on a per-particle base. However, mass items may be declared as the overall emitted amount, i.e. the amount is split among all released particles. This is especially useful if you change the number of particles as the released amount will be independent on the number of particles. On the other hand, the released amount can be specified on a per-particle base.

Similarly the amount of mass items can be declared to be handled as flux or instantaneous release.

NOTE: The interpretation of the values depends on the combined settings for the mass components and number of release particles.

Individual state variables
Each state variable/ class item can be configured separately. The format can be either

- Constant
- Varying in time
- Within range
- Normal distribution
- Discrete distribution

If the format is set to constant or time varying, every particle will receive the specified values, in case of a time series read from a time series data file (dfs0). If the format is one of the following settings, each individual particle will receive an individual value.

Within range
Value uniformly distributed between given Min and Max values.

Normal distribution
Value from a normal distribution with given mean and standard deviation.

Discrete distribution
Value determined from the specified discrete distribution.
A discrete distribution is characterised by a number of bins. Each bin has a certain width and an associated value. The "width" determines the "proportion" or probability for this bin and that a particle will receive the associated value. The width can be a direct scale (i.e. number of items in that bin) or a probability. The value has to be given in the correct item unit.

File Source

Currently only initial sources are supported as file source. In this case the file source specification acts as a hotstart file source, i.e. particle count and coordinates/states are read from a file. This information is used to generate an initial particle distribution where all particle states from a previous run are

restored from a data file. Therefore, besides the data file specification, no other user input is required. Valid data files must contain all internal particle states and can be generated by saving particle data as hotstart track. If a hot-start track contains just one single timestep the date setting of the file is irrelevant. If it contains more than one time step the stored period must cover the whole simulation period. The storage frequency should match the simulation time step, as no data interpolation is performed. In case of a mismatch, the last matching time step in data file is used what could let to unexpected results.

5.15   Initial Conditions

The initial conditions are the spatial distribution of the component concentration throughout the computational domain at the beginning of the simulation. Initial conditions must always be provided. The initial conditions can be the result from a previous simulation in which case the initial conditions effectively act as a hot start of the concentration field for each state variable.

It is currently not possible to specify initial conditions for particle classes. Initial conditions can only be specified for normal state variables.

The initial conditions are specified individually for each state variable.

Data

The format of the initial concentration (in component unit) for the state variable can be specified as

- Constant (in domain)
- Varying in domain

For the case with varying in domain you have to prepare a data file containing the concentration (in component unit) before you set up the hydrodynamic simulation.If the state variable is defined as 2D, the file must be a 2D unstructured data file (dfsu) or a 2D grid data file (dfs2). If the state variable is defined as 3D, the file must be a 3D unstructured data file (dfsu) or a 3D grid data file (dfs3). The area in the data file must cover the model area. If a dfsu-file is used the mesh in the data file must match exactly the mesh in the simulation. If a dfs2-file or a dfs3-file is used, a bilinear interpolation is used to map the data. In case the input data file contains a single time step, this field is used. In case the file contains several time steps, e.g. from the results of a previous simulation, the actual starting time of the simulation is used to interpolate the field in time. Therefore the starting time must be between the start and end time of the file.

5.16   Boundary Conditions

Boundary conditions are only valid for AD-state variables (concentrations). If a particle leaves the domain it is lost and can not re-enter the simulation. Initially, the set-up editor scans the mesh file for boundary codes (sections), displays the recognized codes and suggest a default name for each.You can rename these names to more meaningful names in the Domain dialog.

Depending on the choice of property page you can get a geographic view or a list view of the boundaries.

The specification of the individual boundary information for each code (section) and each component is made subsequently. From the list view you can go to the dialog for specification by clicking the "Go to.." button.

5.16.1   Boundary specification

You can choose between the following three boundary types

- Land
- Specified values (Dirichlet boundary condition)
- Zero gradient (Neumann boundary condition).

Data

If specified values (Dirichlet boundary condition) is selected, the format of the concentration (in component unit) for the AD state variable at the boundary can be specified as

- Constant (in time and along boundary)
- Varying in time and constant along boundary
- Varying in time and along boundary

For the case with boundary data varying in time but constant along the boundary you have to prepare a data file containing the concentration (in component unit) before you set up the hydrodynamic simulation. The data file must be a time series file (dfs0). The data must cover the complete simulation period. The time step of the input data file does not, however, have to be the same as the time step of the hydrodynamic simulation. You can choose between different types of interpolation (see Interpolation type).

For the case with boundary data varying both in time and along the boundary you have to prepare a data file containing the concentration (in component unit) before you set up the hydrodynamic simulation. The data file must be a dfs2 file or a 2D dfsu file containing information from a vertical plane. The data must cover the complete simulation period. The time step of the input data file does not, however, have to be the same as the time step of the

hydrodynamic simulation. You can choose between different types of time interpolation.

Interpolation type

For the two cases with values varying in time two types of time interpolation can be selected:

- Linear
- Piecewise cubic

In the case with values varying along the boundary two methods of mapping from the input data file to the boundary section are available:

- Normal
- Reverse order

Using normal interpolation, the first and last point of the line are mapped to the first and the last node along the boundary section and the intermediate boundary values are found by linear interpolation. Using reverse order interpolation, the last and first point of the line are mapped to the first and the last node along the boundary section and the intermediate boundary values is found by linear interpolation.

Soft start interval

You can specify a soft start interval during which boundary values are increased from a specified reference value to the specified boundary value in order to avoid shock waves being generated in the model. The increase can either be linear or follow a sinusoidal curve.

5.17 Hydrodynamic Conditions

If the Hydrodynamic Module is not included in the simulation you have to provide the flow information using these settings. The MIKE ECO Lab module will then run in a so called stand-alone mode, using an external flow field. The flow information can be read from both unstructured (dfsu) or gridded (dfs2/dfs3) data files. The data files need to cover the model area and span over the entire simulation period. The flow information will be interpolated into the domain mesh, i.e. it can be based on a different (coarser) resolution than the actual domain mesh. If a dfsu-file is used, a piecewise constant interpolation is used to map the data. If a dfs2-file is used, a bilinear interpolation is used to map the data

3D setup (Mike3)
For a 3D setup you have to provide 2 data files. The 2D/area data file must provide the surface elevation. If the bathymetry is not constant during the simulation period (i.e. morphological changes) the file also has to provide the

still water depth. The flow field is read from the 3D/volume data. This volume file must provide the U-, V- and W- components.

5.18   Temperature

The temperature can be specified as

- Not included
  The model assumes a default value for the whole model domain

- User specified temperature

- From hydrodynamic model
  The data calculated in the hydrodynamic module is used directly
  (This option is not available when running a stand-alone setup)

5.18.1   User specified temperature

With a user specified setting, the data can be:

- Constant

- Varying in time, constant in domain

- Varying in time and domain

For the case with values varying in domain you have to prepare a data file containing the information before you set up the hydrodynamic simulation. The file must be a 2D unstructured data file (dfsu) or a 2D grid data file (dfs2). The area in the data file must cover the model area. If a dfsu-file is used, a piecewise constant interpolation is used to map the data. If a dfs2-file is used, a bilinear interpolation is used to map the data

5.19   Salinity

The salinity can be specified as

- Not included
  The model assumes a default value for the whole model domain

- User specified salinity

- From hydrodynamic model
  The data calculated in the hydrodynamic module is used directly
  (This option is not available when running a stand-alone setup)

5.19.1   User specified salinity

With a user specified setting, the data can be:

- Constant

- Varying in time, constant in domain

- Varying in time and domain

For the case with values varying in domain you have to prepare a data file containing the information before you set up the hydrodynamic simulation. The file must be a 2D unstructured data file (dfsu) or a 2D grid data file (dfs2). The area in the data file must cover the model area. If a dfsu-file is used, a piecewise constant interpolation is used to map the data. If a dfs2-file is used, a bilinear interpolation is used to map the data

5.20   Density

The density can be specified as

- Not included
  The model assumes a default value for the whole model domain

- User specified density

- From hydrodynamic model
  The data calculated in the hydrodynamic module is used directly
  (This option is not available when running a stand-alone setup)

5.20.1   User specified density

With a user specified setting, the data can be:

- Constant

- Varying in time, constant in domain

- Varying in time and domain

For the case with values varying in domain you have to prepare a data file containing the information before you set up the hydrodynamic simulation. The file must be a 2D unstructured data file (dfsu) or a 2D grid data file (dfs2). The area in the data file must cover the model area. If a dfsu-file is used, a piecewise constant interpolation is used to map the data. If a dfs2-file is used, a bilinear interpolation is used to map the data

5.21   Output

Standard data files with computed results from the simulation can be specified here. Because result files tend to become large, it is normally not possible to save the computed discrete data in the whole area and at all time steps. In practice, sub areas and subsets must be selected.

In the main outputs dialog you can add a new output file by clicking on the "New output" button. By selecting a file in the Output list and clicking on the

"Delete output" you can remove this file. For each output file you can specify the name (title) of the file and whether the output file should be included or not. The specification of the individual output files is made subsequently. You can go to the dialog for specification by clicking on the "Go to .." button. Finally, you can view the results using the relevant MIKE Zero viewing/editing tool by clicking on the "View" button during and after the simulation.

5.21.1 Geographic view

This shows the geographical position of the output data.

5.21.2 Output Specification

For each selected output file the field type, the output format, the data type, the treatment of flood and dry, the output file (name, location and file type) and time step must be specified. Depending on the output format and data type the geographical extend of the output data must also be specified.

Field type

For a 3D simulation both 2D and 3D field parameters can be selected. If the model definition contains state variables, the mass budget for a domain and the discharge through a cross section can also be selected. If the model definition includes particle classes, particle track, particle hotstart data track and particle track mass budget for can be selected as well.

Output format

The possible choice of output format depends on the specified field type.

For 2D field variables the following formats can be selected

- Point series. Selected field data in geographical defined points.
- Lines series. Selected field data along geographical defined lines.
- Area series. Selected field data in geographical defined areas.

For 3D field variables the following formats can be selected

- Point series. Selected field data in geographical defined points.
- Lines series. Selected field data along geographical defined lines.
- Vertical plane series. Selected field data along geographical defined vertical plane.
- Volume series. Selected field data in geographical defined areas.

If mass budget is selected for the field type, you have to specify the domain for which the mass budget should be calculated. The file type will be a dfs0 file.

If discharge is selected for the field type, you have to specify the cross section through which the discharge should be calculated. The file type will be a dfs0 file.

If particle track is selected for the field type, you have to specify the domain within which the particle tracks should be saved. The track can be written using various track storage formats, see Particle file format page 96.

If particle track mass budget is selected for the field type, you have to specify the domain for which the mass budget should be calculated. The file type will be a dfs0 file.

If particle hotstart data track is selected for the field type, you have to specify the domain within which the particle tracks should be saved. Hotstart data tracks are intended to be used as data file for a file source (hotstart) (see File Source, page 48) and contain additional internal data states compared to standard particle tracks. The track can be written using various track storage formats, see Particle file format page 96, with the constrains that the track format must be a readable format (currently .xml and .track).

Data type

You must specify the data type. You can select discrete values or interpolated values. For point series, area series and volume series both options are available. For line series only interpolated values is available. See also Table 5.1.

If "discrete values" is selected for the data type, the values written in the data file are the cell-averaged values.

If "interpolated values" is selected for the data type, the values written in the data file are determined by 2nd order interpolation. The element in which the point is located is determined and the point value is obtained by linear interpolation using the vertex (node) values for the actual element. The vertex values are calculated from on the cell-averaged values using the pseudo-Laplacian procedure proposed by Holmes and Connell (1989).

Note, that all adjacent elements, including dry elements, are considered in the interpolation calculation.

Output file

A name and location of the output file must be specified along with the file type. The file type depends on the Output format and the Data type as shown in Table 5.1.

Vectors components and tensors components in a 2D dfsu file and horizontal vector components in a 3D dfsu file are given in the projection coordinate system. In a dfs2 file and a dfs3 file the vector and tensor components are given in the local coordinate system.

Table 5.1   List of file types for the output files

Output format	Data type	File type
Point series	Discrete values	dfs0
	Interpolated values	dfs0
Line series	Interpolated values	dfs1
Area series	Discrete values	dfsu, dfs2*
	Interpolated values	dfs2
Vertical plane series	Discrete values	dfsu
	Interpolated values	dfs2
Volume series	Discrete values	dfsu
	Interpolated values	dfs3
Cross-section	Not relevant	dfs0
Domain series	Not relevant	dfs0

* For area series with discrete values selected for the data type the file type dfs2 can only be specified when the Mesh and bathymetry is specified using a bathymetry data file.

Table 5.2   List of tools for viewing, editing and plotting results

File type	Viewing/editing tools	Plotting tools
dfs0	Time Series Editor	Plot Composer
dfs1	Profile Series Editor	Plot Composer Result Viewer
dfs2	Grid Series Editor Data Viewer	Plot Composer Result Viewer Data Viewer
dfs3	Grid Series Editor	Plot Composer Result Viewer
dfsu	Data Viewer Data Manager	Data Viewer Result Viewer Plot Composer (2D)

Particle file format

Particle tracks may be stored in various storage formats. Figure 5.3 lists an overview of the available format options. Most formats store the complete particle track data, i.e. coordinates and variable values for a time step. Some formats store only selected information like particle counts or statistics. Track formats can in general be used by the MIKE software to visualise and post-process particle information. Here the data base format offers fast access[1], whereas XML storage offers easy data access. KML files are for visualizing particle tracks in Google Earth. The various ASCII/csv formats can be used for data exchange with 3rd party tools. If data is written out as individual dfs0 file (one for each particle) the particle class and number is appended to the specified file name. Additionally, a file with the specified name is generated that corresponds to the particle count output, i.e. lists the active number of particles per timestep.

Table 5.3   The different formats for storing particle data

Format	Description	File type
XML particle track (compressed/uncom-pressed)	Particle data stored as XML data	xml
Particle Track database	Particle data stored as binary data-base	track
KML table particle track	Google Earth visualisation	kml
TXT table particle track	Particle data as simple ASCII/csv data table	txt
Particle count	Number of active particles in the domain in every timestep, saved as ASCII/csv or dfs0 file	txt / dfs0
Track info	Particle class information only saved as ASCII/csv, no individual particle data	txt
Dfs0 Particle track	Particle data is saved as individual dfs0 file for every particle	dfs0
Particle track statistics	Some general statistics for particle classes and individual particles	txt

NOTE: Outputs generating plain text files should not be used when utilizing MPI parallelization as the individual sub-domain information cannot automatically be combined. The result file will thus only contain the master domain data. In this case a standard track (xml or track file type) should be written. These can be post-processed using the Particle toolbox to convert into the needed output format.

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1   On the file first access a data index will be added/generated, i.e. the file will grow in size, but subsequent data access will use this index and is much faster.

If a particle hotstart track is generated, i.e. the particle information is intended to be used as a data file for a file source, only a subset of the formats in Table 5.3 are suitable. Currently these are the .xml and .track formats.

Particle tracks in XML and binary format can be used within MIKE Zero in the Plot Composer (Grid Plot/Dfsu Plot), Grid Editor, Result Viewer and Data Viewer where you can add it as a layer to visualize particle movements (right click "Add/Remove Layers..."). The KML format cannot be used within MIKE Zero; its purpose is for displaying data in Google Earth.

Particle track files can get very large, and therefore it is possible only include a subset of particles and time steps in the output file (see Particle numbers page 98). Typically, the binary file for a track is smaller than the XML file, which is smaller than the KML file. Also, the compressed XML file will be smaller than the uncompressed XML file.

Note that the 'Particle Track Tool' in the 'Oil Spill Particle Track Tools Toolbox' contains the functionality to convert a particle track in XML format into other formats such as compressed/uncompressed XML, simple ascii table or dfs0 file format, including the option of filtering the output items.

For each time timestep, the variables for each particle is written in the particle track file. XML and binary files store the xyz coordinates, mass and additional variables (see Output Items page 103). KML files store the longitude-latitude coordinates for viewing the particle track on a map. Further, the z coordinate, mass and additional variables are also saved and can be displayed in Google Earth in the Elevation Profile.

XML files come in two variants: compressed and uncompressed.

- In uncompressed format the values of the xyz-coordinates and each selected variable are saved on separate lines in the file

- In compressed format the values of the xyz-coordinates and each selected variable are saved in the same line in the file

```
<Particle Nr="51">
<x>1079.511942</x>
<y>1017.705602</y>
<z>-0.9754099093</z>
<age>3120.000000</age>
<Mass>60.00000000</Mass>
</Particle>
```

Figure 5.1   Example of data in XML file using uncompressed particle format

```
<Particle Nr="51">
<![CDATA[1079.511942,1017.705602,-0.9754099093,3120.000000,60.00000000]]>
</Particle>
```

Figure 5.2   Example of data in XML file using compressed particle format

Flood and dry

For 2D and 3D field parameters the flood and dry can be treated in three different ways

- Whole area
- Only wet area
- Only real wet area

Selecting the only wet area option the output file will contain delete values for land points. The land points are defined as the points where the water depth is less than a drying depth. When selecting the only real wet area option the output file will contain delete values for points where the water depth is less than the wetting depth. The drying depth and the wetting depth are specified on the Flood and Dry dialog. If flooding and drying is not included both the flooding depth and the wetting depth are set to zero.

Time step

The temporal range refers to the time steps specified under "Simulation Period" in the Time dialog.

If checking the "Use simulation end time" check box, then the simulation end time specified in the Time dialog will automatically be used as last output time step. Hence, the last output time step will be automatically updated if the simulation period is changed.

Particle numbers

The range of the particle numbers refer to the particles ID's in each class. During the simulation all new particles are given an ID. The first particle number is 1 and the total number of particles are the multipla of the overall time step and the number of particles released per time step in each class.

The xml file can get very large, and therefore it is possible not to write particle variables for all particles, but only a fraction of the total number of particles, by selecting a frequency higher than 1.

Point series

You must select the map projection (Long/Lat, UTM-32, etc.) in which you want to specify the horizontal location of the points.

The geographical coordinates of the points are either taken from the dialog or from a file. The file format is an ascii file with four space separated items for each point on separate lines. The first two items must be floats (real numbers) for the x- and y-coordinate. For 3D field data the third item must be an integer for the Layer number if discrete values are selected and a float (real number) for the z-coordinate if interpolated values are selected. The layers

are numbered 1 at the bed and increasing upwards. For 2D field data the third item is unused (but must be specified). The last item (the remaining of the line) is the name specification for each point

Layer number

The layer number selected for discrete values in the point output is defined from the lowest active layer (=1) increasing upwards. In case the mesh is a type sigma mesh, the number of active layers in the water column will always be the same in any point in the domain. In case the mesh is a combined sigma-z level mesh, the number of active layers may vary in the domain. An example is shown in Figure 5.3.
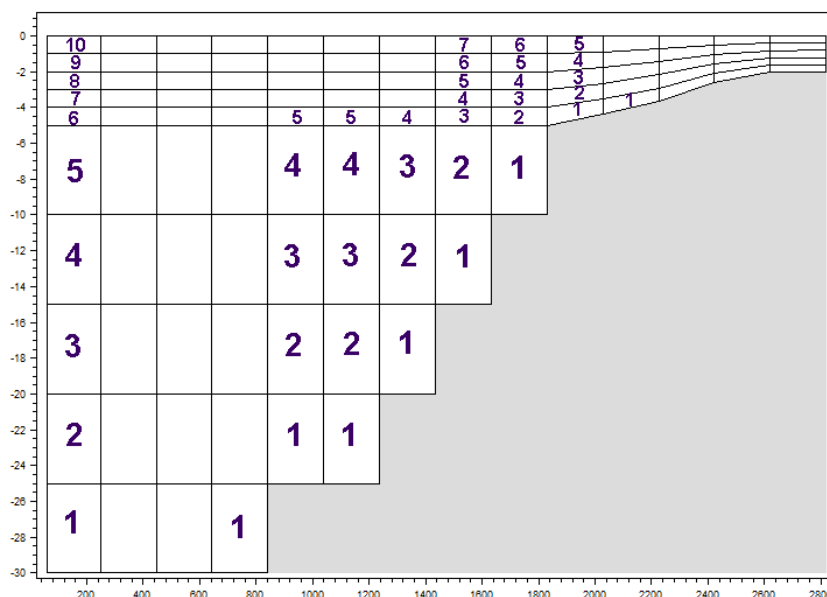

Figure 5.3   Example of layer numbers in point output specification in case of combined sigma-z level mesh.

Line series

You must select the map projection (Long/Lat, UTM-32, etc.) in which you want to specify the horizontal spatial information.

The line is defined by defining a polyline in the horizontal domain. The polyline is given by a number of geo-referenced points. A minimum of two points is required. The polyline is composed of a sequence of line segments. The line segments are straight lines between two successive points. The geographical coordinates are taken from the dialog or from a file. The file format is an ascii file with three space separated items for each of the points on separate lines. The first two items must be floats (real numbers) for the x- and y-coordinate (Easting and Northing or Longitude and Latitude). For 3D field

data the third item must be a float (real number) for the z-coordinate. For 2D field data the third item is unused (but must be specified).

Note: If spherical coordinates (map projection LONG/LAT) is used for a 3D model simulation, the line must be either a horizontal or a vertical line.

Area series

You must select the map projection (Long/Lat, UTM-32, etc.) in which you want to specify the horizontal spatial information.

If discrete values is selected for the data type the discrete field data within a polygon can be selected. The closed region is bounded by a number of line segments. You must specify the coordinates of the vertex points of the polygon. Two successive points are the endpoints of a line that is a side of the polygon. The first and final point is joined by a line segment that closes the polygon. The geographical coordinates of the polygon points are taken from the dialog or from a file. The file format is an ascii file with three space separated items for each of the two points on separate lines. The first two items must be floats (real numbers) for the x- and y-coordinate. The third item is unused (but must be specified).

If interpolated values is selected for the data type the values is calculated on a structured grid (overlay). For each direction you should specify

- The origin
- The grid spacing
- The number of grid points

Furthermore, the orientation of the grid at the origin must be specified. This is defined as the angle between y-axis in the selected projection and the y-axis of the grid measured clockwise.

Vertical plane series

You must select the map projection (Long/Lat, UTM-32, etc.) in which you want to specify the horizontal spatial information.

The vertical plane is defined by defining a polyline in the horizontal domain. The polyline is given by a number of geo-referenced points. A minimum of two points is required. The polyline is composed of a sequence of line segments. The line segments are straight lines between two successive points. The geographical coordinates are taken from the dialog or from a file. The file format is an ascii file with three space separated items for each of the points on separate lines. The first two items must be floats (real numbers) for the x- and y-coordinate (Easting and Northing or Longitude and Latitude). The third item is not used (but must be specified).

If discrete values is selected for the data type you must also specify the range of layers (first and last Layer number) which should be stored in the output file The intersection between the line segments and the faces of the unstructured mesh is determined and added to the list of points on the polyline. A vertical unstructured mesh is then created from the horizontal polyline points and the vertical discretization for the computational mesh. For each element of the of vertical mesh the discrete value at the centroid is determined as the discrete value in the element of the computational mesh, where the centroid point is located.

If interpolated values is selected for the data type the values is calculated on a structured grid (overlay). You should specify the number of grid points along the polyline. For the vertical direction the minimum and maximum z value and the number of grid points should be specified.

In the dfs2 output file Dimension 1 is the coordinate along the polyline and Dimension 2 is the vertical coordinate (z-direction). The origin in the z-direction in the dfs2 file is determined as the specified maximum z value.

Layer number
The layer number(s) selected for the vertical plane output refer to the vertical discretization specified on the Vertical Mesh page. Here the layers are numbered 1 at the lowest layer and increase upwards. In case of a combined sigma-z level mesh only the active elements are saved in the output.

Volume series

You must select the map projection (Long/Lat, UTM-32, etc.) in which you want to specify the horizontal spatial information.

If discrete values is selected for the data type the discrete field data within a polygon can be selected. The closed region is bounded by a number of line segments. You must specify the coordinates of the vertex points of the polygon. Two successive points are the endpoints of a line that is a side of the polygon. The first and final point is joined by a line segment that closes the polygon. The geographical coordinates of the polygon points are taken from the dialog or from a file. The file format is an ascii file with three space separated items for each of the two points on separate lines. The three items must be floats (real numbers) for the x-, y- and z-coordinate. You must also specify the range of layers (first and last Layer number) which should be stored in the output file.

If interpolated values is selected for the data type the values is calculated on a structured grid (overlay). For each direction you should specify

- The origin
- The grid spacing
- The number of grid points

Furthermore, the orientation of the grid at the origin must be specified. This is defined as the angle between y-axis in the selected projection and the y-axis of the grid measured clockwise.

Note, the origin, $z0_{dfs3}$, in the z-direction in the dfs3 file is determined as $z0_{dfs3} = z0 + dz*(nz-1)$, where $z0$ is the user specified origin, dz is the grid spacing and nz in the number of grid points.

Layer number

The layer number(s) selected for the volume output refer to the vertical discretization specified on the Vertical mesh page. Here the layers are numbered 1 at the lowest layer and increase upwards. In case of a combined sigma-z level mesh only the elements containing water are saved in the output. An example is shown in Figure 5.4.
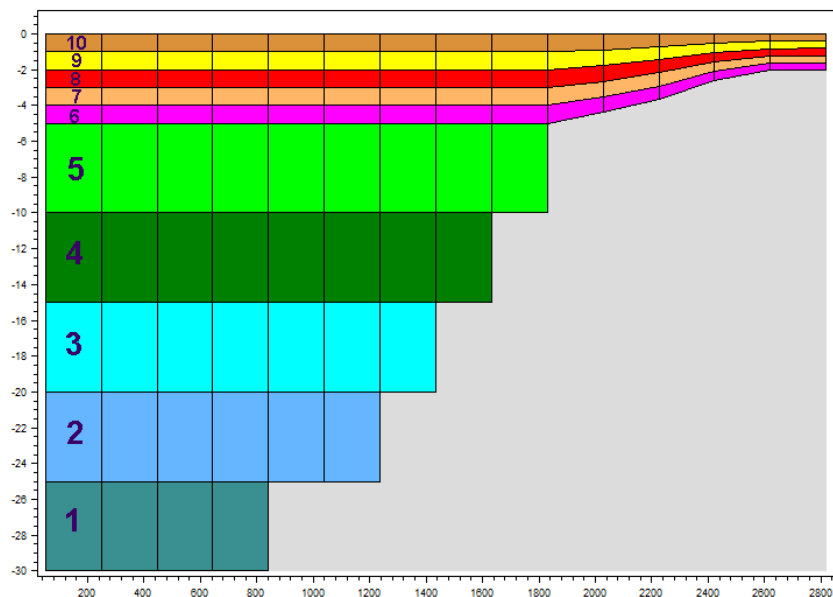

Figure 5.4   Example of layer numbers in volume output specification in case of combined sigma-z level mesh.

Cross section series

The cross section is defined by defining a polyline in the horizontal domain. The polyline is given by a number of geo-referenced points which together make up a polyline. A minimum of two points is required. The polyline is composed of a sequence of line segments. The line segments are straight lines between two successive points. The geographical coordinates are taken from the dialog or from a file. The file format is an ascii file with three space separated items for each of the two points on separate lines. The first two items must be floats (real numbers) for the x- and y-coordinate. The third item is

unused (but must be specified). The polyline (cross section) in the numerical calculations is defined as a section of element faces. The face is included in the section when the line between the two element centres of the faces crosses one of the line segments. The faces defining the cross section are listed in the log-file.

You must also select the map projection (LONG/LAT, UTM-32, etc.) in which you want to specify the horizontal location of the points.

Domain series

The domain for which mass budget should be calculated is specified as a polygon in the horizontal domain. The closed region is bounded by a number of line segments. You must specify the coordinates of the vertex points of the polygon. Two successive points are the endpoints of a line that is a side of the polygon. The first and final point is joined by a line segment that closes the polygon. The geographical coordinates of the polygon points are taken from the dialog or from a file. The file format is an ascii file with three space-separated items for each of the two points on separate lines. The first two items must be floats (real numbers) for the x- and y-coordinate. The third item is unused (but must be specified).

You must also select the map projection (LONG/LAT, UTM-32, etc.) in which you want to specify the horizontal location of the points.

5.21.3 Output Items

Depending on the output type various output items are available. The user can specify a selection of written output items. For outputs of different type than "Mass budget" or "Discharge" one can also select among some predefined output specifications of the active output type from the output library. You can also invoke the output library by pressing the library button.

Field variables

You can select the state variables and the additional variables to be included in the output file. The list of additional variables is specified in the MIKE ECO Lab template and can be

- Auxiliary variables
- Processes
- Derived output

If the chosen template defines particle classes it is also possible to select particle attributes for

- State variables
- Derived variables

The hydraulic variables like velocity components are also included in the list of additional variables.

You can include/exclude all variables of a category by the control element in the lower left corner of the dialog. Note that these check boxes are tri-state elements, i.e. when some elements of a category are included and some excluded the check box shows an intermediate state.

The "write" column allows you to specify that the current, instantanous value or some static data (min, max, average in time etc.) will be saved.

In the "handle" column you can specify that the data will be handled normally or that it will be converted into a mass (total sum), an area concentration (total sum divided by cell area) or a volume concentration (total mass divided by cell volume). For particle attributes the default handling depends on the attribute's type. For mass and concentration attributes the total mass/concentration will be calculated, for other attribute types the average cell value will be used.

Both statistic values and data handling are only supported for MIKE ECO Lab variables and particle attributes.

Depending on the output type particle attributes from all suspended, sedimented or particles within a defined z-Range can be selected as own category.

Mass budget

You can select the mass budget calculation to be included for the flow and for the AD state variables (state variables which are transported by the advection-dispersion). For each selected component the following items are included in the output file

- Total area - total volume/energy/mass within polygon

- Wet area - volume/energy/mass in the area within polygon for which the water depth is larger than the drying depth.

- Real wet area - volume/energy/mass in the area within polygon for which the water depth is larger than the wetting depth

- Dry area - volume/energy/mass in the area within polygon for which the water depth is less than the drying depth

- Transport - accumulated volume/energy/mass transported over lateral limits of polygon

- Source - accumulated volume/energy/mass added/removed by sources within polygon

- Process - accumulated volume/energy/mass added/removed by processes within polygon

- Error - accumulated volume/energy/mass error within polygon determined as the difference between the total mass change and the accumulated mass due to transport, sources and processes

The accumulated volume/mass error contains the contribution due to correction of the transported component when the values become larger than the specified maximum value or lower than the specified minimum value.

For temperature the relative energy (relative to the energy at 0 ºC), E (J), in a volume of water V (m^3) is calculated by

$$E = c_{water}\rho_{water}T \cdot V \qquad (5.18)$$

where T (ºC) is the temperature, c_{water} = 4217.0 J/(K·kg) is the specific heat for water and ρ_{water} = 1010.0 kg/m^3 is the density of water.

For salinity the mass of salt, M (kg), in a volume of water V (m^3) is calculated by

$$M = \rho_{water}S \cdot V / 1000 \qquad (5.19)$$

where S (PSU) is the salinity and ρ_{water} = 1010.0 kg/m^3 is the density of water.

Discharge

You can select the discharge calculation to be included for the flow and the AD state variables (state variables which are transported by the advection-dispersion). Each selected component will result in a number of output items.

You can select between two types of output items:

- Basic
- Extended

The basic output items are as follows:

- Discharge - volume/energy/mass flux through the cross section
- Acc. discharge - accumulated volume/energy/mass flux through the cross section

The extended output items that are included in the output file in addition to the basic output items are as follows:

- Positive discharge
- Accumulated positive discharge
- Negative discharge
- Accumulated negative discharge

By definition, discharge is positive for flow towards left when positioned at the first point and looking forward along the cross-section line. The transports are always integrated over the entire water depth.

For temperature the relative energy (relative to the energy at 0 ºC), E (J), in a volume of water V (m³) is calculated by

$$E = c_{water}\rho_{water}T \cdot V \tag{5.20}$$

where T (ºC) is the temperature, c_{water} = 4217.0 J/(K·kg) is the specific heat for water and ρ_{water} = 1010.0 kg/m³ is the density of water.

For salinity the mass of salt, M (kg), in a volume of water V (m³) is calculated by

$$M = \rho_{water}S \cdot V/1000 \tag{5.21}$$

where S (PSU) is the salinity and ρ_{water} = 1010.0 kg/m³ is the density of water.

Particle track

If your model includes a particle class definition you can select to write out the attributes of the particles to various track storage formats. Apart from the state variables and derived variables defined by the particle class you may also output some generic information such as the age since the release of a particle and the movement parameters (horizontal direction and speed, vertical speed) used for the latest movement of the particle.

For each selected particle the following items can be included in the output file

- State variables
- Derive variables
- Age
- Horizontal speed
- Horizontal direction
- Vertical speed

If a particle hotstart track is generated no use selectable output items are available.

Particle track mass budget

You can select the mass budget calculation to be included for the particles. For each selected class component the following items are included in the output file

- Suspended active/current - mass of particles in area within polygon that is into suspension

- Suspended accumulated - accumulated mass of particles in area within polygon that has been into suspension

- Sedimented active/current - mass of particles in area within polygon that is settling on seabed

- Sedimented accumulated - accumulated mass of particles in area within polygon that has settled on seabed

- Released active/current - mass of particles in area within polygon that is released within polygon

- Released accumulated - accumulated mass of particles in area within polygon that has been released within polygon

- Stranded active/current - mass of particles in area within polygon that is stranding on dry land

- Stranded accumulated - accumulated mass of particles in area within polygon that has stranded on dry land

The output library

The output library can be used to maintain different predefined output item selections, i.e. user defined sets of output items for various output types. A single selection of output items is called an output set. Such sets can be stored (and retrieved) from individual files, so called output collections. The output library consist of at least one or more such collections.

The default collection is the initial values collection and represents the parameterisation of the initially loaded setup. It is neither possible to add nor to remove this default collection or to add/delete sets to it. The main purpose of the initial collection is be able to revert to the initial states stored in the setup. To add a new, user defined collection use the "new" button and specify the storage location and file name in the following dialogue. Please note that existing files will be overwritten without further notice! The "load" button can be used to open an existing output collection file, i.e. make all stored output item selections available in the available definition list (see load output definition). 'The "unload" button will remove the access to selected collection and all its sets but will not delete the collection file.

To add the current active output item specifications of the setup, select the collection and press the "add" button. This will append the collection and add a new output item set. You can specify a name and a short description text for both the collection and for each stored set that will be used to identify a specific set. To update an existing set with the current settings, select the set and use the "update" button. This will overwrite the stored specifications with the current values from the setup.

To leave the parameter set library use the "close" or "save and close" buttons. The later will write any new/updated set (marked with a "*" in front of their name) to the specified collection files.

6   LIST OF REFERENCES

/1/   Holmes, D. G. and Connell, S. D. (1989), Solution of the 2D Navier-Stokes on unstructured adaptive grids, AIAA Pap. 89-1932 in Proc. AIAA 9th CFD Conference.

/2/   Rodi, W. (1980), Turbulence Models and Their Application in Hydraulics - A State of the Art Review, *Special IAHR Publication*.

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